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CONDENSED MATTER PHYSICS

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INTRODUCTION

NOTES

Condensed matter physics is the field of physics that deals with the macroscopic and microscopic physical properties of matter, especially the solid and liquid phases which arise from electromagnetic forces between atoms. More generally, the subject deals with 'Condensed' phases of matter: systems of many constituents with strong interactions between them. More exotic condensed phases include the superconducting phase exhibited by certain materials at low temperature, the ferromagnetic and antiferromagnetic phases of spins on crystal lattices of atoms, and the Bose–Einstein condensate found in ultracold atomic systems. Condensed matter physicists seek to understand the behaviour of these phases by experiments to measure various material properties, and by applying the physical laws of quantum mechanics, electromagnetism, statistical mechanics, and other theories to develop mathematical models.

Theoretical condensed matter physics involves the use of theoretical models to understand properties of states of matter. These include models to study the electronic properties of solids, such as the band structure, the density functional theory, etc. Experimental condensed matter physics involves the use of experimental probes to try to discover new properties of materials. Such probes include effects of electric and magnetic fields, measuring response functions, transport properties and thermometry.

The diversity of systems and phenomena available for study makes condensed matter physics the most active field of contemporary physics. The field overlaps with chemistry, materials science, engineering and nanotechnology, and relates closely to atomic physics and biophysics. The theoretical physics of condensed matter shares important concepts and methods with that of particle physics and nuclear physics.

This book, *Condensed Matter Physics*, is divided into four blocks, which are further subdivided into fourteen units. This book provides a basic understanding of the subject and helps to grasp its fundamentals. In a nutshell, it explains crystalline solids, crystal lattice and crystal structure, ordered phase of matter, space lattice, unit cell and primitive cell, Bravais lattice, crystal systems, type of lattices (SC, BCC, FCC, HCP), Miller indices, Wigner-Seitz cells, lattice vibrations, electrical properties of metals, free electron gas in three dimensions, Fermi energy, Hall effect, Kronig-Penney model, semiconductors, polarization, Clausius-Mossotti relation, Lorentz field, dielectric constant, polarizability, electronic, ionic, Piezo, Pyro and Ferro electric properties of crystals, classification of magnetic materials, Langevin's theory of paramagnetism, quantum theory of paramagnetism, ferromagnetism, Weiss molecular field theory, antiferromagnetism, Neel's theory, ferrimagnetism and ferrites, superconductivity – experimental survey, Meissner effect, type I and type II superconductors, superconductivity – theoretical survey,

London equations, coherence length, BCS theory, Cooper pair, normal tunnelling and Josephson effect, and high temperature superconductors.

The book follows the Self-Instructional Mode (SIM) wherein each unit begins with an 'Introduction' to the topic. The 'Objectives' are then outlined before going on to the presentation of the detailed content in a simple and structured format. 'Check Your Progress' questions are provided at regular intervals to test the student's understanding of the subject. 'Answers to Check Your Progress Questions', a 'Summary', a list of 'Key Words', and a set of 'Self-Assessment Questions and Exercises' are provided at the end of each unit for effective recapitulation.

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BLOCK - I
CRYSTAL STRUCTURE AND LATTICES

NOTES

UNIT 1 CRYSTAL STRUCTURE

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1.0 INTRODUCTION

In physics especially in crystallography, crystal structure is a description of the ordered arrangement of atoms, ions or molecules in a crystalline material. Ordered structures occur from the intrinsic nature of the constituent particles to form symmetric patterns that repeat along the principal directions of 3-dimensional space in matter.

Crystal structure is described in terms of the geometry of arrangement of particles in the unit cell. The unit cell is defined as the smallest repeating unit having the full symmetry of the crystal structure. The geometry of the unit cell is defined as a parallelepiped, providing six lattice parameters taken as the lengths of the cell edges (a, b, c) and the angles between them (á, â, ã). The positions of particles inside the unit cell are described by the fractional coordinates (x_i, y_i, z_i) along the cell edges, measured from a reference point. It is only necessary to report the coordinates of a smallest asymmetric subset of particles. This group of particles may be chosen so that it occupies the smallest physical space, which means that not all particles need to be physically located inside the boundaries given by the lattice parameters. All other particles of the unit cell are generated by the symmetry operations that characterize the symmetry of the unit cell. The collection of symmetry operations of the unit cell is expressed formally as the space group of the crystal structure.

The crystal structure and symmetry play a critical role in determining many physical properties, such as cleavage, electronic band structure, and optical transparency.

NOTES

In this unit, you will study about the crystalline solids, crystal lattice, crystal structure, symmetry elements, and ordered phase of matter.

1.1 OBJECTIVES

After going through this unit, you will be able to:

- Define the crystalline solids
- Understand the crystal lattice
- Explain the crystal structure
- Comprehend the symmetry elements
- Analyse the ordered phase of matter

1.2 CLASSIFICATION OF SOLIDS

If we examine the solid materials with which we daily come across, we shall find that most of them do not have any characteristic difference in their outward appearance. But, if we examine them under a microscope we shall find that these materials have different internal atomic structures.

Based on the internal atomic structure, the solids can be classified into two categories, namely, (*i*) *Crystalline* and (*ii*) *Non-Crystalline or Amorphous Solids.*

1.3 CRYSTALLINE SOLIDS (CRYSTALS)

Crystalline solids or crystals are those in which the constituent atoms or molecules are arranged in an orderly fashion throughout in a three dimensional pattern.

Each atom or molecule is fixed at a definite point in space at a definite distance from and in a definite angular orientation to all other atoms or molecules surrounding it. Therefore, crystalline solids have well-defined geometrical form (pattern), i.e., they have well-defined faces and angles between them.

[In a crystal, the atoms are arranged like soldiers on a parade ground in well defined columns and rows.]

Further when crystal breaks, the broken pieces have regular shapes. *The crystalline solids have directional properties and therefore they are called anisotropic substances.*

A crystalline material may be either in the form of a single crystal (where the solid contains only one crystal) or an aggregate of many small crystals or grains separated by well defined grain boundaries (***also known as polycrystalline solid***).

Few examples for crystalline solids: Copper, Silver, Aluminium, Iron, etc.

Crystallography: *The study of the geometric form and other physical properties of crystalline solids by using X-rays, electron beams and neutron beams, etc., is termed as the science of crystallography.*

Note:
- ***Grains***: The crystals are also known grains.
- ***Grain Boundary***: The boundary separating the two adjacent grains is called grain boundary.
- ***Whisker***: Whiskers are nothing but artificially produced crystals. They are produced under some special conditions so that they do not have any structure defects.
- ***Examples for Single Crystals***: Sugar, common salt (NaCl), diamond, etc. These single crystals are produced artificially from their vapour or liquid state.

1.4 AMORPHOUS SOLIDS (NON-CRYSTALLINE SOLIDS)

'Amorphous' means 'Without Form'

In amorphous solids, the constituent particles, atoms or molecules are not arranged in an orderly fashion, i.e., the same atomic groups are arranged more randomly.

These solids have no directional properties and therefore they are called isotropic substances. These amorphous solids do not have a sharp melting point.

Examples: Plastics, Rubber and Glass.

Note:
- ***Supercooled Liquids***
  The materials like glass, which exhibit some of the properties of a solid like hardness, definite shape, etc., but are not crystalline, are regarded as supercooled liquids.

Check Your Progress

1. Define the classification of solids.
2. What are the crystalline solids (crystals)?
3. Explain the term crystallography.
4. Elaborate on the whisker.
5. Interpret the amorphous solids (non-crystalline solids).
6. What do you understand by the supercooled liquids?

1.5 CRYSTAL STRUCTURE

NOTES

The crystal structure gives the arrangement and disposition of atoms within a crystal. *Determination of crystal structure with the help of X-rays is known as X-ray crystallography.*

X-rays are most widely used to study the crystal structure because the wavelength of X-rays (10^{-12} to 10^{-10} m) is most comparable with the inter-atomic distances.

Fundamental Crystallographic Terms (Definitions)

1. Lattice

Lattice is defined as an array of points such that every lattice point has got the same environment or every point is indistinguishable from the other lattice point.

It is an imaginary concept.

2. Space Lattice or Crystal Lattice

Definition 1: A three-dimensional collection of points in space is called a space lattice or crystal lattice. The environment about any particular point is in every way the same.

Definition 2: A geometrical representation of the crystal structure in terms of lattice points is called space lattice, provided the environment about every point is identical to that of every other point.

That is, space lattice is an idealised geometrical (imaginary) concept by which crystal structures can be described.

Explanation: We know that a metal consists of a number of crystals, and each crystal, in turn, consists of a large number of atoms.

Consider the cross-section of a crystal, in which the atoms be arranged in a rectangular pattern, as shown in Figure 1.1.

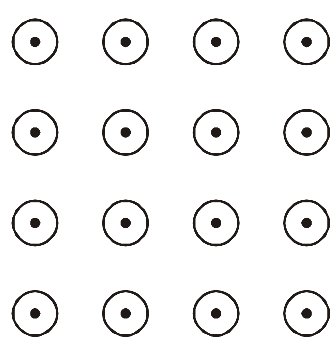


Fig. 1.1 *Arrangement of Atoms (Cross-Section of a Metal Crystal)*

From the Figure 1.2 it may be noted that each atom present in the crystal has its surroundings identical to that of every other atom. Now, if we replace all the atoms in this cross section by points (corresponding to the centres of all atoms), then the resulting collection of points shown in Figure 1.2 is called a ***lattice***. This is the case of a two-dimensional lattice or *plane lattice.*

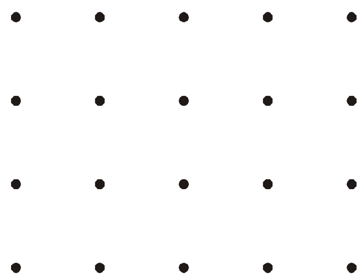


Fig. 1.2 *Plane Lattice*

Similarly, the group of lattice points in the three-dimensional pattern is known as crystal lattice or space lattice.

It may be noted that in a crystal lattice, each point has its surrounding identical to that of every other point.

Lattice Points

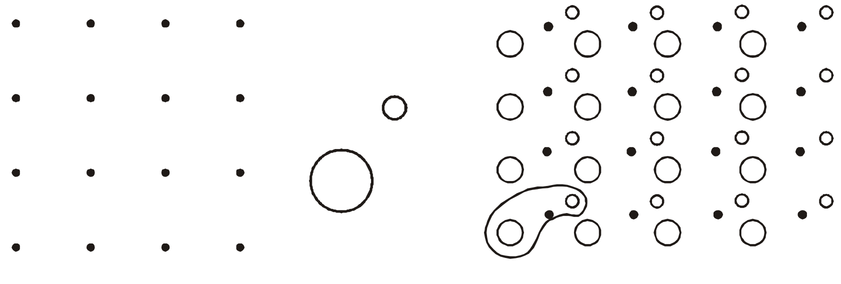
Definition 1: Lattice points denote the position of atoms or molecules in the crystal.

Definition 2: The points in the space lattice are called lattice points.

Basis or Motif

A crystal structure is formed by associating with every lattice point a unit assembly of atoms or molecules (*i.e., one or more atoms or molecules*) *that are identical in composition, arrangement and orientation. This unit assembly is called the basis or pattern or motif* (*Refer Figure 1.3*).

The logical relation is, Space Lattice + Basis = Crystal Structure



(a) Lattice *(b) Basis* *(c) Crystal Structure—the crystal structure is formed by the addition of basis Figure (b) to every lattice point of the lattice Figure (a)*

Fig. 1.3 *Crystal Structure*

NOTES

The number of atoms in the basis may be as low as 1. Example, aluminium and barium. In NaCl and KCl the basis is two atoms and in CaF_2 the basis is three atoms. But, there are structures for which the basis exceeds 1,000 atoms.

Note: • A crystal lattice refers to the geometry of a set of points in space whereas the crystal structure refers to the actual ordering or alignments of its constituent ions, atoms or molecules in the space.

Lattice Planes

A set of parallel and equally spaced planes in a space lattice which include all lattice points are called lattice planes.

The different ways of drawing the lattice planes for the array of Figure 1.3 is shown in Figure 1.4.

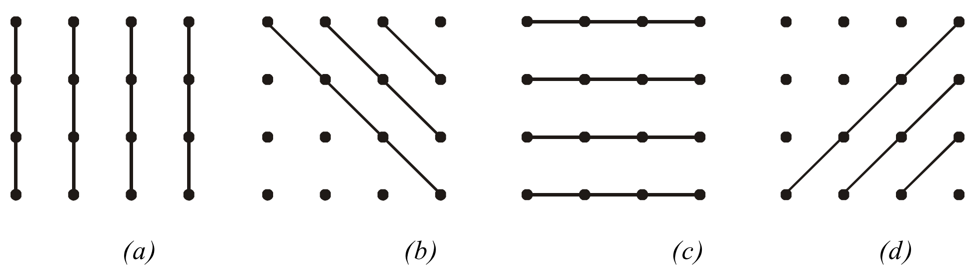


Fig. 1.4 *The Different Ways of Drawing Lattice Planes*

Unit Cell

Definition 1: The unit cell is defined as the smallest geometric figure, the repetition of which gives the actual crystal structure.

Definition 2: It may also be defined as the fundamental elementary pattern of minimum number of atoms, molecules or groups of molecules which represent fully all the characteristics of the unit cell.

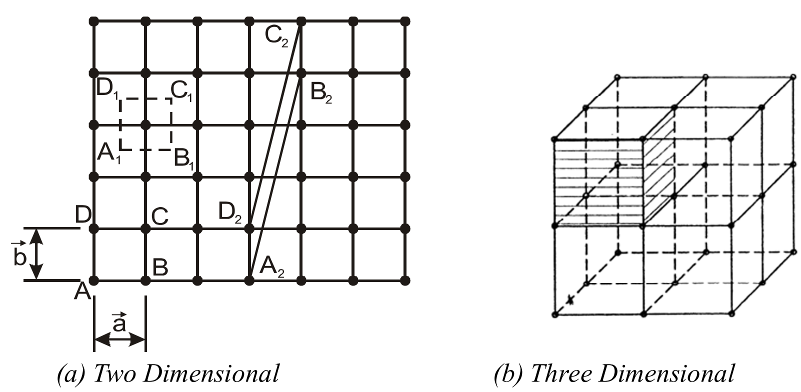


Fig. 1.5 *Unit Cell*

Consider a two-dimensional crystal lattice shown in Figure 1.5. When a parallelogram such as ABCD is rotated repeatedly by any integral multiple of vectors $\vec{a}, \vec{b}$, then corresponding to AB and AD whole pattern or array may be obtained. The whole crystal may thus be reproduced.

This region ABCD is called a unit cell and $\vec{a},\vec{b}$ the basis vectors.

The choice of a unit cell is ***not unique***. But, it can be constructed into a number of ways like $A_1 B_1 C_1 D_1$ or $A_2 B_2 C_2 D_2$ without affecting the symmetry of the crystal.

NOTES

We can extend the same procedure for a three dimensional case also. Figure 1.5 shows the unit cell in three dimension.

Definition: A unit cell in three dimension is defined as that volume of the solid from which the entire crystal can be formed by the translational repetition in three dimension.

Note:
- The unit cell may be considered as the brick of a wall where the latter represents the crystal. We know that the shape of the wall depends upon the shape and arrangement of the brick. Similarly, the shape of the crystal will depend upon the shape of the unit cell and the arrangement of atoms within the unit cell.
- ***Translation:*** Motion of a body in which all the points in the body follow parallel paths.
- ***Other terms used to represent a unit cell:*** The unit cell is also known as basic cell or basic unit or fundamental unit or fundamental elementary pattern or building block or lattice unit.

Lattice Parameters

Figure 1.6 shows a unit cell of a three-dimensional crystal lattice.

The lines drawn parallel to the lines of intersection of any three faces of the unit cell, which do not lie in the same plane, are called crystallographic axes.

The intercepts a, b and c are nothing but the edges of the unit cell (i.e., the distance between two lattice points), which defines the dimensions of an unit cell. *These intercepts are known as its primitives or characteristic intercepts along the axes.*

These three quantities a, b and c are also *called the fundamental translational vectors.* The angles between (a, b), (b, c) and (c, a) are denoted by γ, α and β, respectively. *The three angles (α, β and γ) are called interfacial angles.*

Both the intercepts and interfacial angles constitute the lattice parameters of the unit cell.

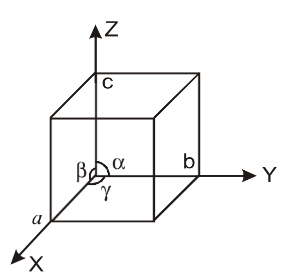


Fig. 1.6 *Lattice Parameters*

The form and actual size of the unit cell can be determined if the values of intercepts and interfacial angles are known.

Primitive Cell (P)

NOTES

A primitive cell is the simplest type of unit cell which contains one lattice point per unit cell (contains lattice points at its corner only).

Example: Cubic Cell.

If there are more than one lattice point it is called a non-primitive cell.

Example: BCC and FCC contain more than one lattice point per unit cell.

If the number of lattice points per unit cell is two (BCC), three and four (FCC) the unit cell is called **doubly primitive, triply primitive** and **quadruply primitive, respectively.**

1.6 SYMMETRY ELEMENTS

A symmetry element is a point of reference about which symmetry operations can take place. In particular, symmetry elements can be identities, mirror planes, axes of rotation (both proper and improper), and centres of inversion. A symmetry element corresponds to a symmetry operation that generates the same representation of an object. The identity symmetry element is found in all objects and is denoted E. It corresponds to an operation of doing nothing to the object.

Mirror planes are denoted by σ. In particular, a vertical mirror plane is denoted σ_v. Rotational symmetry, also known as radial symmetry, is represented by an axis about which the object rotates in its corresponding symmetry operation. A group of proper rotations is denoted as C_n, where n is the order of rotation. The C_n notation is also used for the related, more abstract, cyclic group. An improper rotation is the composition of a rotation about an axis and a reflection in a plane perpendicular to that axis. Its group is denoted by S_n.

For inversion, denoted i, there must be a point in the centre of an object that is the inversion centre. In the inversion operation for 3*D* coordinates, the inversion centre is the origin (0,0,0). When an object is inverted, the position vector of a point in an object, è'*x*,*y*,*z*é', is inverted to è'-*x*,-*y*,-*z*é'.

1.7 ORDERED PHASE OF MATTER

The terms order and disorder entitle the presence or absence of some symmetry or correlation in a many-particle systems. The exact form of order in a solid is lattice periodicity. Lattice periodicity implies long-range order. The common states of matter, namely solid, liquid and gas are differs mainly by the types and degrees of order present in the phase. These states of matter, however, are not sufficient to characterize the structures found in all systems.

NOTES

Some substances shows intermediate states having less order than solids, but possessing more order than liquids. These intermediate state of partially ordered fluids known as liquid crystal state.

Crystalline solids molecules are ordered in both the ways, namely- Positional Order and Orientational Order. They subjugate specific locations in a lattice. Thus, a crystal has orientational and three dimensional positional order. Each of these parameters describes the extent to which the crystal sample is ordered.

Positional order refers to the extent to which an average molecule or group of molecules shows translational symmetry. Orientational order represents a measure of the tendency of the molecules to align along the axis in crystalline solid.

Check Your Progress

7. Explain the term crystal structure.
8. What do you mean by the lattice?
9. Define the space lattice or crystal lattice.
10. Illustrate the unit cell.
11. Elaborate on the primitive cell.
12. Interpret the symmetry elements.
13. Explain the ordered phase of matter.

1.8 ANSWERS TO CHECK YOUR PROGRESS QUESTIONS

1. Based on the internal atomic structure, the solids can be classified into two categories, namely, (i) Crystalline and (ii) Non-Crystalline or Amorphous Solids.
2. Crystalline solids or crystals are those in which the constituent atoms or molecules are arranged in an orderly fashion throughout in a three dimensional pattern.
3. The study of the geometric form and other physical properties of crystalline solids by using X-rays, electron beams and neutron beams, etc., is termed as the science of crystallography.
4. Whiskers are nothing but artificially produced crystals. They are produced under some special conditions so that they do not have any structure defects.
5. 'Amorphous' means 'Without Form'. In amorphous solids, the constituent particles, atoms or molecules are not arranged in an orderly fashion, i.e., the same atomic groups are arranged more randomly.
6. The materials like glass, which exhibit some of the properties of a solid like hardness, definite shape, etc., but are not crystalline, are regarded as supercooled liquids.

NOTES

7. The crystal structure gives the arrangement and disposition of atoms within a crystal. Determination of crystal structure with the help of X-rays is known as X-ray crystallography.
8. Lattice is defined as an array of points such that every lattice point has got the same environment or every point is indistinguishable from the other lattice point.
9. A three-dimensional collection of points in space is called a space lattice or crystal lattice. The environment about any particular point is in every way the same.
10. The unit cell is defined as the smallest geometric figure, the repetition of which gives the actual crystal structure. It may also be defined as the fundamental elementary pattern of minimum number of atoms, molecules or groups of molecules which represent fully all the characteristics of the unit cell.
11. A primitive cell is the simplest type of unit cell which contains one lattice point per unit cell (contains lattice points at its corner only).
12. A symmetry element is a point of reference about which symmetry operations can take place. In particular, symmetry elements can be identities, mirror planes, axes of rotation (both proper and improper), and centres of inversion.
13. The terms order and disorder entitle the presence or absence of some symmetry or correlation in a many-particle systems. The exact form of order in a solid is lattice periodicity.

1.9 SUMMARY

- Based on the internal atomic structure, the solids can be classified into two categories, namely, (i) Crystalline and (ii) Non-Crystalline or Amorphous Solids.
- Crystalline solids or crystals are those in which the constituent atoms or molecules are arranged in an orderly fashion throughout in a three dimensional pattern.
- The study of the geometric form and other physical properties of crystalline solids by using X-rays, electron beams and neutron beams, etc., is termed as the science of crystallography.
- Whiskers are nothing but artificially produced crystals. They are produced under some special conditions so that they do not have any structure defects.
- 'Amorphous' means 'Without Form'. In amorphous solids, the constituent particles, atoms or molecules are not arranged in an orderly fashion, i.e., the same atomic groups are arranged more randomly.
- The materials like glass, which exhibit some of the properties of a solid like hardness, definite shape, etc., but are not crystalline, are regarded as supercooled liquids.

- The crystal structure gives the arrangement and disposition of atoms within a crystal. Determination of crystal structure with the help of X-rays is known as X-ray crystallography.
- Lattice is defined as an array of points such that every lattice point has got the same environment or every point is indistinguishable from the other lattice point.
- A three-dimensional collection of points in space is called a space lattice or crystal lattice. The environment about any particular point is in every way the same.
- The unit cell is defined as the smallest geometric figure, the repetition of which gives the actual crystal structure. It may also be defined as the fundamental elementary pattern of minimum number of atoms, molecules or groups of molecules which represent fully all the characteristics of the unit cell.
- A primitive cell is the simplest type of unit cell which contains one lattice point per unit cell (contains lattice points at its corner only).
- A symmetry element is a point of reference about which symmetry operations can take place. In particular, symmetry elements can be identities, mirror planes, axes of rotation (both proper and improper), and centres of inversion.
- The terms order and disorder entitle the presence or absence of some symmetry or correlation in a many-particle systems. The exact form of order in a solid is lattice periodicity.

1.10 KEY WORDS

- **Crystalline solids:** Crystalline solids or crystals are those in which the constituent atoms or molecules are arranged in an orderly fashion throughout in a three dimensional pattern.
- **Crystallography:** The study of the geometric form and other physical properties of crystalline solids by using X-rays, electron beams and neutron beams, etc., is termed as the science of crystallography.
- **Grains:** The crystals are also known grains.
- **Grain boundary:** The boundary separating the two adjacent grains is called grain boundary.
- **Whisker:** Whiskers are nothing but artificially produced crystals. They are produced under some special conditions so that they do not have any structure defects.
- **Lattice:** Lattice is defined as an array of points such that every lattice point has got the same environment or every point is indistinguishable from the other lattice point.
- **Lattice points:** Lattice points denote the position of atoms or molecules in the crystal.

NOTES

- **Unit cell:** The unit cell is defined as the smallest geometric figure, the repetition of which gives the actual crystal structure.
- **Primitive cell:** A primitive cell is the simplest type of unit cell which contains one lattice point per unit cell (contains lattice points at its corner only).

1.11 SELF ASSESSMENT QUESTIONS AND EXERCISES

Short-Answer Questions

1. Explain the classification of solids.
2. Define the term crystallography.
3. Illustrate the amorphous solids (non-crystalline solids).
4. What do you mean by the supercooled liquids?
5. Elaborate on the crystal structure.
6. Interpret the space lattice or crystal lattice.
7. Define the primitive cell.
8. Explain the symmetry elements.
9. What is the ordered phase of matter?

Long-Answer Questions

1. Discuss briefly the classification system of solids.
2. Analyse the crystal structure with the help of examples.
3. Discuss in detail about the fundamental crystallographic terms.
4. Explain the symmetry elements. Give appropriate examples.
5. Describe the ordered phase of matter.

1.12 FURTHER READINGS

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UNIT 2 CRYSTAL SYSTEM

NOTES

Structure

2.0 Introduction
2.1 Objectives
2.2 Translation and Orientation Order
2.3 Space Lattice
2.4 Unit Cell
2.5 Primitive Cell (P)
2.6 The Crystal System and Bravais Lattice
2.7 Answers to Check Your Progress Questions
2.8 Summary
2.9 Key Words
2.10 Self Assessment Questions and Exercises
2.11 Further Readings

2.0 INTRODUCTION

In condensed matter physics, the terms crystal system refer to one of several classes of space groups, lattices, point groups, or crystals. Informally, two crystals are in the same crystal system if they have similar symmetries, although there are many exceptions to this.

Crystal systems, crystal families, and lattice systems are similar but slightly different, and there is widespread confusion between them: in particular the trigonal crystal system is often confused with the rhombohedral lattice system, and the term “Crystal System” is sometimes used to mean “Lattice System” or “Crystal Family”.

In a crystal system, a set of point groups and their corresponding space groups are assigned to a lattice system. Of the 32 point groups that exist in three dimensions, most are assigned to only one lattice system, in which case both the crystal and lattice systems have the same name. However, five point groups are assigned to two lattice systems, rhombohedral and hexagonal, because both exhibit threefold rotational symmetry. These point groups are assigned to the trigonal crystal system. In total there are seven crystal systems: triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal, and cubic.

Space groups and crystals are divided into seven crystal systems according to their point groups, and into seven lattice systems according to their Bravais lattices. Five of the crystal systems are essentially the same as five of the lattice systems, but the hexagonal and trigonal crystal systems differ from the hexagonal and rhombohedral lattice systems. The six crystal families are formed by combining the hexagonal and trigonal crystal systems into one hexagonal family, to eliminate this confusion.

In this unit, you will study about the translation and orientation order, space lattice, unit cell, primitive cell, Bravais lattice, and crystal systems.

NOTES

2.1 OBJECTIVES

After going through this unit, you will be able to:

- Understand the translation and orientation order
- Comprehend the space lattice
- Explain the unit cell and primitive cell
- Define Bravais lattice and crystal systems

2.2 TRANSLATION AND ORIENTATION ORDER

A translation is a geometric transformation that moves every point of a figure or a space by the same distance in a given direction. A translation can also be interpreted as the addition of a constant vector to every point, or as shifting the origin of the coordinate system. In a Euclidean space, any translation is an isometry.

Often, vertical translations are considered for the graph of a function. If f is any function of x, then the graph of the function $f(x) + c$ (whose values are given by adding a constant c to the values of f) may be obtained by a vertical translation of the graph of $f(x)$ by distance c. For this reason the function $f(x) + c$ is sometimes called a vertical translate of $f(x)$. For instance, the anti-derivatives of a function all differ from each other by a constant of integration and are therefore vertical translates of each other.

In condensed matter physics, translational motion is movement that changes the position of an object, as opposed to rotation. For example, according to Whittaker:

"If a body is moved from one position to another, and if the lines joining the initial and final points of each of the points of the body are a set of parallel straight lines of length –!, so that the orientation of the body in space is unaltered, the displacement is called a translation parallel to the direction of the lines, through a distance –!."

— E. T. Whittaker: A Treatise on the Analytical Dynamics of Particles and Rigid Bodies

A translation is the operation changing the positions of all points (x, y, z) of an object according to the formula

$$(x, y, z) \to (x + \Delta x, y + \Delta y, z + \Delta z)$$

Where $(\Delta x,\ \Delta y,\ \Delta z)$, is the same vector for each point of the object. The translation vector $(\Delta x,\ \Delta y,\ \Delta z)$ common to all points of the object

describes a particular type of displacement of the object, usually called a linear displacement to distinguish it from displacements involving rotation, called angular displacements.

NOTES

Orientation order signifies a measure of the tendency of the molecules to align along the director on a long-range basis. Bond orientation order describes a line joining the centres of nearest-neighbour molecules without requiring a regular spacing along that line.

Thus, orientation order denotes the level or degree to which the molecules align along a specific direction on a long-range basis. In a crystalline solid, molecules are ordered in both the above.

2.3 SPACE LATTICE

Space lattices also referred to as Bravais lattices, describe the geometric arrangement of the lattice points, and therefore the translational symmetry of the crystal. The three dimensions of space afford 14 distinct Bravais lattices describing the translational symmetry. All crystalline materials recognized today, not including quasi-crystals, fit in one of these arrangements.

A Bravais lattice, named after Auguste Bravais (1850), is an infinite array of discrete points generated by a set of discrete translation operations described in three dimensional space by:

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

Where the n_i are any integers and a_i are primitive vectors which lie in different directions and span the lattice. The choice of primitive vectors for a given Bravais lattice is not unique. A fundamental aspect of any Bravais lattice is that, for any choice of direction, the lattice will appear exactly the same from each of the discrete lattice points when looking in that chosen direction.

The Bravais lattice concept is used to formally define a crystalline arrangement and its (finite) frontiers. A crystal is made up of a periodic arrangement of one or more atoms (the basis or motif) at each lattice point. The basis may consist of atoms, molecules, or polymer strings of solid matter. Two Bravais lattices are often considered equivalent if they have isomorphic symmetry groups. In this sense, there are 14 possible Bravais lattices in three-dimensional space. The 14 possible symmetry groups of Bravais lattices are 14 of the 230 space groups. In the context of the space group classification, the Bravais lattices are also called Bravais classes, Bravais arithmetic classes, or Bravais flocks.

A three-dimensional collection of points in space is called a space lattice or crystal lattice. The environment about any particular point is in every way the same. On the other hand, A geometrical representation of the crystal structure in terms of lattice points is called space lattice, provided the environment about every point is identical to that of every other point. That is, space lattice is an idealised

geometrical (imaginary) concept by which crystal structures can be described. Similarly, the group of lattice points in the three-dimensional pattern is known as crystal lattice or space lattice.

NOTES

The crystal structure consists of the same group of atoms, the basis, positioned around each and every lattice point. This group of atoms therefore repeats indefinitely in three dimensions according to the arrangement of one of the Bravais lattices. The characteristic rotation and mirror symmetries of the unit cell is described by its crystallographic point group.

2.4 UNIT CELL

The smallest group of particles in the material that constitutes this repeating pattern is the unit cell of the structure. The unit cell completely reflects the symmetry and structure of the entire crystal, which is built up by repetitive translation of the unit cell along its principal axes. The translation vectors define the nodes of the Bravais lattice.

The lengths of the principal axes, or edges, of the unit cell and the angles between them are the lattice constants, also called lattice parameters or cell parameters. The symmetry properties of the crystal are described by the concept of space groups. All possible symmetric arrangements of particles in three-dimensional space may be described by the 230 space groups.

Crystal structure is described in terms of the geometry of arrangement of particles in the unit cell. The unit cell is defined as the smallest repeating unit having the full symmetry of the crystal structure. The geometry of the unit cell is defined as a parallelepiped, providing six lattice parameters taken as the lengths of the cell edges (a, b, c) and the angles between them (α, β, γ). The positions of particles inside the unit cell are described by the fractional coordinates (x_i, y_i, z_i) along the cell edges, measured from a reference point. It is only necessary to report the coordinates of a smallest asymmetric subset of particles. This group of particles may be chosen so that it occupies the smallest physical space, which means that not all particles need to be physically located inside the boundaries given by the lattice parameters. All other particles of the unit cell are generated by the symmetry operations that characterize the symmetry of the unit cell. The collection of symmetry operations of the unit cell is expressed formally as the space group of the crystal structure.

There are two special cases of the unit cell: the primitive cell and the conventional cell. The primitive cell is a unit cell corresponding to a single lattice point. In some cases, the full symmetry of a crystal structure is not obvious from the primitive cell, in which cases a conventional cell may be used. A conventional cell (which may or may not be primitive) is the smallest unit cell with the full symmetry of the lattice and may include more than one lattice point.

NOTES

An alternative to the unit cell, for every Bravais lattice there is another kind of cell called the Wigner–Seitz cell. In the Wigner–Seitz cell, the lattice point is at the center of the cell, and for most Bravais lattices, the shape is not a parallelogram or parallelepiped. This is a type of Voronoi cell. The Wigner–Seitz cell of the reciprocal lattice in momentum space is called the Brillouin zone.

2.5 PRIMITIVE CELL (P)

A primitive cell is a unit cell that contains exactly one and only one lattice point. For unit cells generally, lattice points that are shared by *n* cells are counted as $\frac{1}{n}$ of the lattice points contained in each of those cells; so for example a primitive unit cell in three dimensions which has lattice points only at its eight vertices is considered to contain $\frac{1}{8}$ of each of them. An alternative conceptualization is to consistently pick only one of the *n* lattice points to belong to the given unit cell (so the other 1-*n* lattice points belong to adjacent unit cells).

The primitive translation vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$ span a lattice cell of smallest volume for a particular three-dimensional lattice, and are used to define a crystal translation vector

$$\vec{T} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3,$$

Where u_1, u_2, u_3 are integers, translation by which leaves the lattice invariant. That is, for a point in the lattice *r*, the arrangement of points appears the same from $\mathbf{r}' = \mathbf{r} + \vec{T}$ as from $\mathbf{r}$.

Since the primitive cell is defined by the primitive axes (vectors) $\vec{a}_1, \vec{a}_2, \vec{a}_3$ the volume V_p of the primitive cell is given by the parallelepiped from the above axes as,

$$V_p = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$$

Thus, primitive cell is the simplest type of unit cell which contains one lattice point per unit cell (contains lattice points at its corner only). A primitive cell is a unit cell that contains exactly one lattice point. It is the smallest possible cell.

2.6 THE CRYSTAL SYSTEM AND BRAVAIS LATTICE

The terms crystal system refer to one of several classes of space groups, lattices, point groups, or crystals. Informally, two crystals are in the same crystal system if they have similar symmetries, although there are many exceptions to this.

NOTES

In a crystal system, a set of point groups and their corresponding space groups are assigned to a lattice system. Of the 32 point groups that exist in three dimensions, most are assigned to only one lattice system, in which case both the crystal and lattice systems have the same name. However, five point groups are assigned to two lattice systems, rhombohedral and hexagonal, because both exhibit threefold rotational symmetry. These point groups are assigned to the trigonal crystal system. In total there are seven crystal systems: triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal, and cubic.

Crystal systems, crystal families, and lattice systems are similar but slightly different, and there is widespread confusion between them: in particular the trigonal crystal system is often confused with the rhombohedral lattice system, and the term "Crystal System" is sometimes used to mean "Lattice System" or "Crystal Family".

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$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

The Bravais lattice concept is used to formally define a crystalline arrangement and its (finite) frontiers. A crystal is made up of a periodic arrangement of one or more atoms (the basis or motif) at each lattice point. The basis may consist of atoms, molecules, or polymer strings of solid matter. Two Bravais lattices are often considered equivalent if they have isomorphic symmetry groups. In this sense, there are 14 possible Bravais lattices in three-dimensional space. The 14 possible symmetry groups of Bravais lattices are 14 of the 230 space groups. In the context of the space group classification, the Bravais lattices are also called Bravais classes, Bravais arithmetic classes, or Bravais flocks.

Check Your Progress

1. What do you understand by the translation order?
2. Explain the term orientation order.
3. Define the term space lattice.
4. Elaborate on the unit cell.
5. Interpret the primitive cell.
6. State the crystal system.

2.7 ANSWERS TO CHECK YOUR PROGRESS QUESTIONS

1. A translation is a geometric transformation that moves every point of a figure or a space by the same distance in a given direction. A translation can also be interpreted as the addition of a constant vector to every point, or as shifting the origin of the coordinate system. In a Euclidean space, any translation is an isometry.
2. Orientation order signifies a measure of the tendency of the molecules to align along the director on a long-range basis. Bond orientation order describes a line joining the centres of nearest-neighbour molecules without requiring a regular spacing along that line.
3. Space lattices also referred to as Bravais lattices, describe the geometric arrangement of the lattice points, and therefore the translational symmetry of the crystal. The three dimensions of space afford 14 distinct Bravais lattices describing the translational symmetry. All crystalline materials recognized today, not including quasi-crystals, fit in one of these arrangements.
4. The smallest group of particles in the material that constitutes this repeating pattern is the unit cell of the structure. The unit cell completely reflects the symmetry and structure of the entire crystal, which is built up by repetitive translation of the unit cell along its principal axes. The translation vectors define the nodes of the Bravais lattice.
5. The primitive cell is the simplest type of unit cell which contains one lattice point per unit cell (contains lattice points at its corner only). A primitive cell is a unit cell that contains exactly one lattice point. It is the smallest possible cell.
6. The terms crystal system refer to one of several classes of space groups, lattices, point groups, or crystals. Informally, two crystals are in the same crystal system if they have similar symmetries, although there are many exceptions to this.

2.8 SUMMARY

- A translation is a geometric transformation that moves every point of a figure or a space by the same distance in a given direction. A translation can also be interpreted as the addition of a constant vector to every point, or as shifting the origin of the coordinate system. In a Euclidean space, any translation is an isometry.

NOTES

- Orientation order signifies a measure of the tendency of the molecules to align along the director on a long-range basis. Bond orientation order describes a line joining the centres of nearest-neighbour molecules without requiring a regular spacing along that line.
- Space lattices also referred to as Bravais lattices, describe the geometric arrangement of the lattice points, and therefore the translational symmetry of the crystal. The three dimensions of space afford 14 distinct Bravais lattices describing the translational symmetry. All crystalline materials recognized today, not including quasi-crystals, fit in one of these arrangements.
- The smallest group of particles in the material that constitutes this repeating pattern is the unit cell of the structure. The unit cell completely reflects the symmetry and structure of the entire crystal, which is built up by repetitive translation of the unit cell along its principal axes. The translation vectors define the nodes of the Bravais lattice.
- The primitive cell is the simplest type of unit cell which contains one lattice point per unit cell (contains lattice points at its corner only). A primitive cell is a unit cell that contains exactly one lattice point. It is the smallest possible cell.
- The terms crystal system refer to one of several classes of space groups, lattices, point groups, or crystals. Informally, two crystals are in the same crystal system if they have similar symmetries, although there are many exceptions to this.
- Crystal systems, crystal families, and lattice systems are similar but slightly different, and there is widespread confusion between them: in particular the trigonal crystal system is often confused with the rhombohedral lattice system, and the term "Crystal System" is sometimes used to mean "Lattice System" or "Crystal Family".
- The Bravais lattice concept is used to formally define a crystalline arrangement and its (finite) frontiers. A crystal is made up of a periodic arrangement of one or more atoms (the basis or motif) at each lattice point.

2.9 KEY WORDS

- **Translation order:** A translation is a geometric transformation that moves every point of a figure or a space by the same distance in a given direction.
- **Orientation order:** Orientation order signifies a measure of the tendency of the molecules to align along the director on a long-range basis.

- **Space lattice:** Space lattices also referred to as Bravais lattices, describe the geometric arrangement of the lattice points, and therefore the translational symmetry of the crystal.
- **Unit cell:** The unit cell completely reflects the symmetry and structure of the entire crystal, which is built up by repetitive translation of the unit cell along its principal axes.
- **Primitive cell:** A primitive cell is a unit cell that contains exactly one lattice point. It is the smallest possible cell.
- **Crystal systems:** The terms crystal system refer to one of several classes of space groups, lattices, point groups, or crystals.

2.10 SELF ASSESSMENT QUESTIONS AND EXERCISES

Short-Answer Questions

1. Explain the translation order.
2. Define the term orientation order.
3. Elaborate on the space lattice.
4. What do you understand by the unit cell?
5. State the primitive cell.
6. Elucidate on the crystal system.

Long-Answer Questions

1. Briefly discuss the translation and orientation order giving suitable examples.
2. Explain the space lattice with the help of an example.
3. Differentiate between the unit cell and the primitive cell.
4. Analyse the crystal system and Bravais lattice giving examples.

2.11 FURTHER READINGS

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NOTES

UNIT 3 LATTICES

Structure

3.0 Introduction
3.1 Objectives
3.2 Types of Lattices: SC, BCC, FCC
3.3 HCP
3.4 Miller Indices
3.5 Reciprocal Lattice
3.6 Wigner-Seitz Cells
3.7 Bonding in Solids
3.8 Answers to Check Your Progress Questions
3.9 Summary
3.10 Key Words
3.11 Self Assessment Questions and Exercises
3.12 Further Readings

3.0 INTRODUCTION

A lattice is an ordered arrangement of points describing the arrangement of particles that form a crystal. The lattice describes the location and repetitive array of lattice points. Thus, a lattice is a discrete but infinite regular arrangement of points (lattice points) in a vector space.

In condensed matter physics, a lattice model is a physical model that is defined on a lattice, as opposed to the continuum of space or space-time. Lattice models originally occurred in the context of condensed matter physics, where the atoms of a crystal automatically form a lattice.

Currently, lattice models are quite popular in theoretical physics, for many reasons. Some models are exactly solvable, and thus offer insight into physics beyond what can be learned from perturbation theory. Lattice models are also ideal for study by the methods of computational physics, as the discretization of any continuum model automatically turns it into a lattice model.

A lattice system is a class of lattices with the same set of lattice point groups, which are subgroups of the arithmetic crystal classes. The 14 Bravais lattices are grouped into seven lattice systems: triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral, hexagonal, and cubic.

The Wigner–Seitz cell, named after Eugene Wigner and Frederick Seitz, is a primitive cell which has been constructed by applying Voronoi decomposition to a crystal lattice.

NOTES

Solids can be classified according to the nature of the bonding between their atomic or molecular components. The traditional classification distinguishes four kinds of bonding: (i) Covalent bonding, which forms network covalent solids (sometimes called simply "Covalent Solids"), (ii) Ionic bonding, which forms ionic solids, (iii) Metallic bonding, which forms metallic solids, and (iv) Weak inter molecular bonding, which forms molecular solids.

In this unit, you will study about the lattices, types of lattices: SC, BCC, FCC, HCP, the Miller indices, reciprocal lattice, the Wigner-Seitz cells, and the bonding in solids.

3.1 OBJECTIVES

After going through this unit, you will be able to:

- Define the lattices and type of lattices, such as SC, BCC, FCC, and HCP
- Explain the Miller indices
- Understand the reciprocal lattice
- Comprehend the Wigner-Seitz cells
- Illustrate the bonding in solids

3.2 TYPES OF LATTICES: SC, BCC, FCC

We know that the cubic structure is the simplest type of array in which the atoms take positions at the corners of the cube. However, there are three types of lattices possible in this system depending on the positions of the lattice points in the unit cell.

1. Simple Cubic or Primitive (SC or P)
2. Body Centered Cubic (BCC)
3. Face Centered Cubic (FCC)

1. In simple cubic lattice, there is one lattice point at each of the eight corners of the unit cell. The atoms touch along the cube edges as shown in Figure 3.1(a).
2. A Body Centered Cubic (BCC) lattice consists of eight corner atoms, one at each corner and in addition, one atom at the centre of the unit cell, as shown in Figure 3.1(b) called the body centered atom.

NOTES

Table 3.1 *The seven Crystals Systems and their 14 Bravais lattices*

SystemBravais lattice	*Unit cell*	*Characteristic Characteristics*	*Symmetry elements*	*Example*
Cubic	Simple	$a = b = c$	Four 3-fold rotation axes	NaCl, CaF_2, $NaClO_3$
	Body centered	$\alpha = \beta = \gamma = 90°$	(along cube diagonal)	
	Face centered			
Tetragonal	Simple	$a = b \neq c$	One 4-fold rotation axis	$NiSO_4$, SnO_2
	Body centered	$\alpha = \beta = \gamma = 90°$		
Orthorhombic	Simple	$a \neq b \neq c$	Three mutually orthogonal	KNO_3, $BaSO_4$, $MgSO_4$
	Base centered	$\alpha = \beta = \gamma = 90°$	2-fold rotation axes	
	Body centered			
	Face centered			
Monoclinic	Simple	$a \neq b \neq c$	One 2-fold rotation axis	Na_2SO_4, $FeSO_4$
	Base centered	$\alpha = \beta = 90° \neq \gamma$		
Triclinic	Simple	$a \neq b \neq c$	None	$CuSO_4$, $K_2Cr_2O_7$
		$\alpha \neq \beta \neq \gamma \neq 90°$		
Trigonal (Rhombohedral)	Simple	$a = b = c$	One 3-fold rotation axis	$CaSO_4$, calcite
		$\alpha = \beta = \gamma \neq 90°$		
Hexagonal	Simple	$a = b \neq c$	One 3-fold rotation axis	SiO_2, AgI, quartz
		$\alpha = \beta = 90°$		
		$\gamma = 120°$		

NOTES

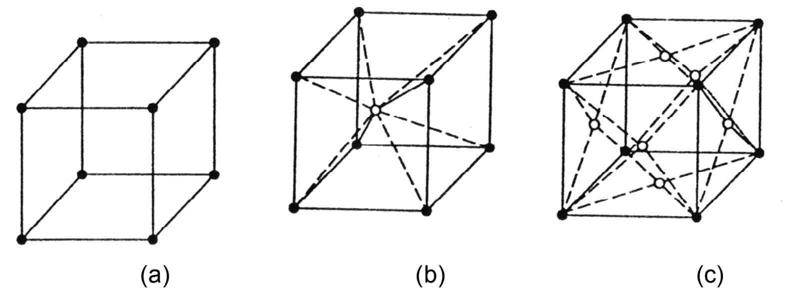


Fig. 3.1 Space Lattices of the Cubic System

3. A face centered cubic (FCC) lattice consists of eight corner atoms, one at each corner and in addition, six atoms, one in each face of the unit cell at the centre of their faces (Figure 3.1(c)).

3.3 HCP

In the hexagonal close packed structure, as shown in Figure 3.2, the unit cell contains one atom at each corner of the two hexagonal prisms (top and bottom), one atom each at the centre of the hexagonal faces and three more atoms within the body of the cell.

It is thus obvious that each unit cell shares 14 atoms and contains 3 full atoms.

The common examples of this type of structure are Magnesium, zinc, zirconium, cadmium, etc.

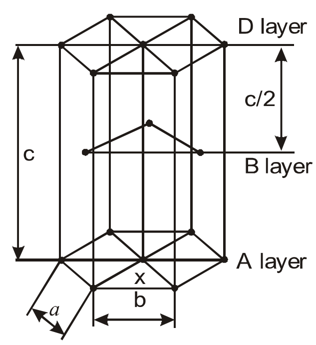


Fig. 3.2 Hexagonal Close Packed Structure

The calculation of coordination number, number of atoms per unit cell, atomic radius and packing factor is explained below.

1. Coordination Number

With reference to Figure 3.3, there are three layers (A, B, D) in the hexagonal system. Consider the bottom A-layer. In this layer, the central atom (x) has six

neighbouring atoms in its own layer. Further at a distance $\frac{c}{2}$ from the bottom A-layer, there are two layers, one is above B-layer and another is below (not shown), containing three atoms in each layer. These layer atoms are also the neighbouring atoms for the reference atom (x). Therefore, the total number of neighbouring atoms are 6 + 3 + 3. Hence, the coordination number is 12.

2. Number of Atoms per Unit Cell

In Figure 3.3, there are six corner atoms at each top D-layer and bottom A-layer. There is one face-centred atom at each top D-layer and bottom A-layer, and three full atoms at the middle layer B-layer of the structure.

Each corner atom is shared by six surrounding hexagon cells.

Therefore, the number of corner atoms in the top layer is $\frac{1}{6} \times 6 = 1$.

Similarly, the number of corner atoms in the bottom layer is $\frac{1}{6} \times 6 = 1$.

Each central atom at the top and bottom layer is shared by two unit cells.

Therefore, the number of centre atoms in the top layer is $\frac{1}{2} \times 1 = \frac{1}{2}$.

Similarly, the number of centre atoms in the bottom layer is $\frac{1}{2} \times 1 = \frac{1}{2}$.

But the three atoms within the body of the cell are fully contributing to the cell, i.e., they are not shared by other unit cells.

Therefore, the total noumber of atoms per unit cell in hexagonal close packed structure is

= Number of corner atoms per unit cell (top and bottom layer) + Number of centre atoms per unit cell (top and bottom layer) + Number of middle layer atoms per unit cell

$$= (1 + 1) + \left(\frac{1}{2} + \frac{1}{2}\right) + 3$$

$$= 2 + 1 + 3 = 6.$$

3. Atomic Radius

To find atomic radius of hcp structure, consider any two corner atoms. It is to be noted that each and every corner atom touches each other (nearest neighbours), as shown in Figure 3.3.

$$\therefore \qquad a = 2r$$

$$\text{Or} \qquad r = \frac{a}{2}$$

Therefore, the atomic radius is $\mathbf{r} = \frac{a}{2}$

NOTES

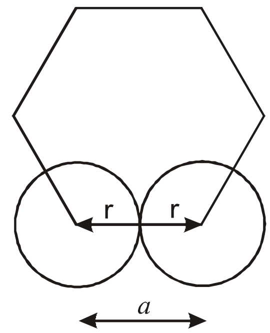


Fig. 3.3

4. Relation between 'c' and 'a' $\left[\frac{c}{a}\text{ ratio}\right]$

In hexagonal system, let the height of the unit cell be c and the distance between two neighbouring atoms be *a*.

In Figure 3.4(a), I, J, K, L, M, N and O are the bottom layer of atoms in hcp structure and P, Q, T are the middle layer atoms.

Consider the arrangement of atoms I, N, O and P shown in Figure 3.4(b). I, N and O represent the bottom layer atoms and P represents the middle layer atom. Now, let us draw the normal line OR from O to the line IN, which bisects the line IN.

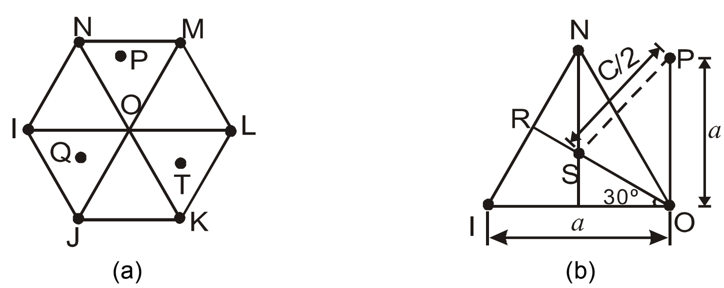


Fig. 3.4 *Arrangement of Atoms in HCP Structure*

Consider a triangle IRO,

$$\cos 30° = \frac{OR}{OI} \text{ or } OR = OI \cos 30°$$

$$OR = a\frac{\sqrt{3}}{2} \qquad [\because OI = a] \qquad ...(3.1)$$

If 'S' is orthocentre, it is found that the length of 'OS' is equal to $\frac{2}{3}$ *of OR.*

NOTES

That is, $$\text{OS} = \frac{2}{3}\ \text{OR}$$

$$\therefore \quad \text{OS} = \frac{2}{3}\, a\, \frac{\sqrt{3}}{2} \qquad \text{[from equation (3.1)]}$$

Or $$\text{OS} = \frac{a}{\sqrt{2}} \qquad ...(3.2)$$

In triangle SOP, $$\text{OP}^2 = \text{OS}^2 + \text{SP}^2 \qquad ...(3.3)$$

Substituting OP, OS and SP values in Equation (3.3), we get,

$$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2 \qquad \left[\because \text{OP} = a \text{ and SP} = \frac{c}{2}\right]$$

On rearranging and simplifying we get,

$$a^2 = \frac{a^2}{3} + \frac{c^2}{4} \quad \text{or} \quad a^2 - \frac{a^2}{3} = \frac{c^2}{4}$$

$$\therefore \quad \frac{2a^2}{3} = \frac{c^2}{4} \quad \text{or} \quad \frac{c^2}{a^2} = \frac{8}{3}$$

Hence, $$\frac{c}{a} = \left(\frac{8}{3}\right)^{\frac{1}{2}} \qquad ...(3.4)$$

Equation (3.4) gives the axial ratio $\left(\frac{c}{a}\right)$ for *a* hcp structure.

5. Atomic Packing Factor (APF)

$$\text{APF} = \frac{\text{Number of atoms per unit cell} \times \text{Volume of one atom}}{\text{Volume of the unit cell}} \qquad ...(3.5)$$

Number of atoms per unit cell in hcp structure = 6.
Therefore, volume of all the atoms in a unit cell =

$$6 \times \frac{4}{3}\pi r^3 = \frac{24}{3}\pi\left[\frac{a}{2}\right]^3 = \pi a^3 \qquad \left[\because r = \frac{a}{2}\right] \qquad ...(3.6)$$

The volume of the unit cell = Area of the base × Height

Area of the base = 6 × Area of the triangle ION

From Figure 3.4(b) area of the triangle

$$\text{ION} = \frac{1}{2}\,(\text{IN})\,(\text{RO}) = \frac{1}{2}\,a \times \frac{a\sqrt{3}}{2} = \frac{a^2\sqrt{3}}{4}$$

NOTES

$$\text{Thus, area of the base} = 6 \times \frac{a^2\sqrt{3}}{4} = \frac{\mathbf{3\sqrt{3}}}{\mathbf{2}}\boldsymbol{a^2}.$$

The height of the hcp structure = c.

Therefore, the volume of the unit cell = Area of the base × Height

$$= \frac{3\sqrt{3}}{2}a^2 \times \text{c} \qquad ...(3.7)$$

Substituting Equations (3.2) and (3.2) in Equation (3.1)

$$\text{APF} = \frac{\pi a^3}{\frac{3\sqrt{3}}{2}a^2\text{c}} = \frac{2\pi}{3\sqrt{3}}\left[\frac{a}{\text{c}}\right] = \frac{2\pi}{3\sqrt{3}}\left[\frac{3}{8}\right]^{\frac{1}{2}} \qquad \left[\because \frac{\text{c}}{a} = \left(\frac{8}{3}\right)^{\frac{1}{2}}\right]$$

$$= \frac{\sqrt{2}\pi}{6} = 0.74$$

Therefore, 74% of the volume is occupied by atoms and the remaining 26% volume is vacant. ***Thus, the packing density is 74%, which is the same as that of FCC structure.***

Table 3.2 *Summary*

System	SC	BCC	FCC	HCP
Atoms per unit cell	1	2	4	6
Coordination number	6	8	12	12
Atomic radius	$\frac{a}{2}$	$\frac{a\sqrt{3}}{4}$	$\frac{a\sqrt{2}}{4}$	$\frac{a}{2}$
Atomic packing factor	$\frac{\pi}{6}$	$\frac{\sqrt{3}\pi}{8}$	$\frac{\sqrt{2}\pi}{6}$	$\frac{\sqrt{2}\pi}{6}$
	0.52	0.68	0.74	0.74

3.4 MILLER INDICES

In a crystal, there exists direction and planes which contain a large concentration of atoms.

Therefore, it is necessary to locate these directions and planes for a crystal to analyse. The problem is how to identify the direction and to designate (to choose) a plane in a crystal.

Here, let us discuss briefly the method of designating a plane in a crystal. This method was suggested by Miller.

Miller Indices

Miller introduced a set of three numbers to designate a plane in a crystal. This set of three numbers is known as Miller indices of the concerned plane.

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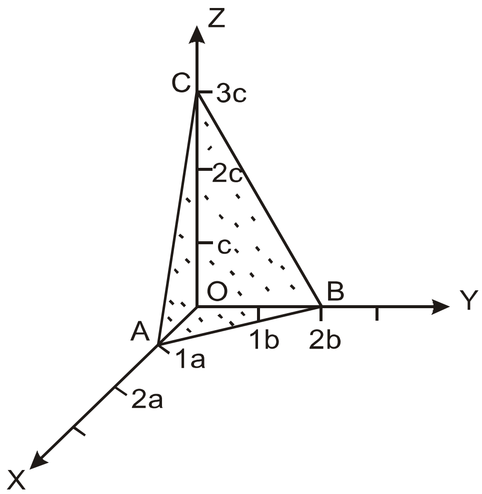


Fig. 3.5 *Crystal Plane*

Procedure for Finding Miller Indices (Steps in the Determination of Miller Indices)

The steps in the determination of Miller indices of a plane are illustrated with the aid of Figure 3.5. Consider the plane ABC which cuts 1 unit along the X-axis, 2 units along the Y-axis and 3 units along the Z-axis.

Step 1:

Find the intercept of the plane ABC along the three axes X, Y and Z. Let it be OA, OB and OC. Express the intercepts in terms of multiples of axial lengths, i.e., lattice parameters. Let them be OA = pa, OB = qb and OC = rc, where p, q and r are the intercept numerical values along the three axis.

In this example,

$p = 1,\ q = 2$ and $r = 3$

Hence, OA : OB : OC = pa : qb : rc = la : 2b : 3c

Therefore, the intercepts are 1a, 2b and 3c along the three axes.

Step 2:

Find the reciprocal of the numerical intercept values, i.e., $\frac{1}{p}\frac{1}{q}\frac{1}{r}$.

For the example shown the reciprocal of the numerical intercept values are

$$\frac{1}{1}\frac{1}{2}\frac{1}{3}.$$

NOTES

Step 3:

Convert these reciprocals into whole numbers by multiplying each with their least common multiple (LCM). In this example the LCM is 6. Therefore,

$$6 \times \frac{1}{1} \qquad 6 \times \frac{1}{2} \qquad 6 \times \frac{1}{3}$$

$$6 \qquad 3 \qquad 2$$

Step 4:

Enclose these numbers in bracket. This represents the indices of the given plane, and is called the Miller indices of the plane. For the example shown, the Miller indices are (6 3 2).

It is generally denoted by (hkl). It can also be noticed that

$$h:k:l = \frac{1}{p}:\frac{1}{q}:\frac{1}{r}.$$

Definition 1: *Thus, Miller indices may be defined as the reciprocal of the intercepts made by the plane along the three crystallographic axes which are reduced to smallest numbers.*

Definition 2: *Miller indices are the three smallest possible integers, which have the same ratio as the reciprocals of the intercepts of the plane concerned along the three axes.*

Note:
- The indices of a plane are represented by a small bracket (hkl). Sometimes, the notations < > and [ ] or { } are also used.
- Negative indices are represented by putting a bar over the digit.

Example : $(1\,\bar{1}\,0), (\bar{1}\,0\,\bar{1})$

Important Features of Miller Indices of Crystal Plane

For the cubic crystal especially, the important features of Miller indices are:

1. For an intercept at infinity, the corresponding index is zero.

   (That is, if a plane is parallel to any one of the coordinate axis, then its intercept is at infinity. Hence, the Miller index for that axis is zero).
2. All equally spaced parallel planes have the same Miller indices (*hkl*) or vice versa.

   (That is, if the Miller indices of two planes have the same ratio like (844), (422) and (211), then the planes are parallel to each other).
3. The indices (*hkl*) do not define a particular plane, but a set of parallel planes.
4. It is only the ratio of the indices which is important in this notation.
5. If a plane cuts the axis on the negative side of the origin, corresponding index is negative.

NOTES

Examples

1. The Miller indices of the plane ABCD, BFGC and AEFB for the Figures 3.6 (a, b and c) are (1 0 0) (0 1 0) and (0 0 1) respectively.

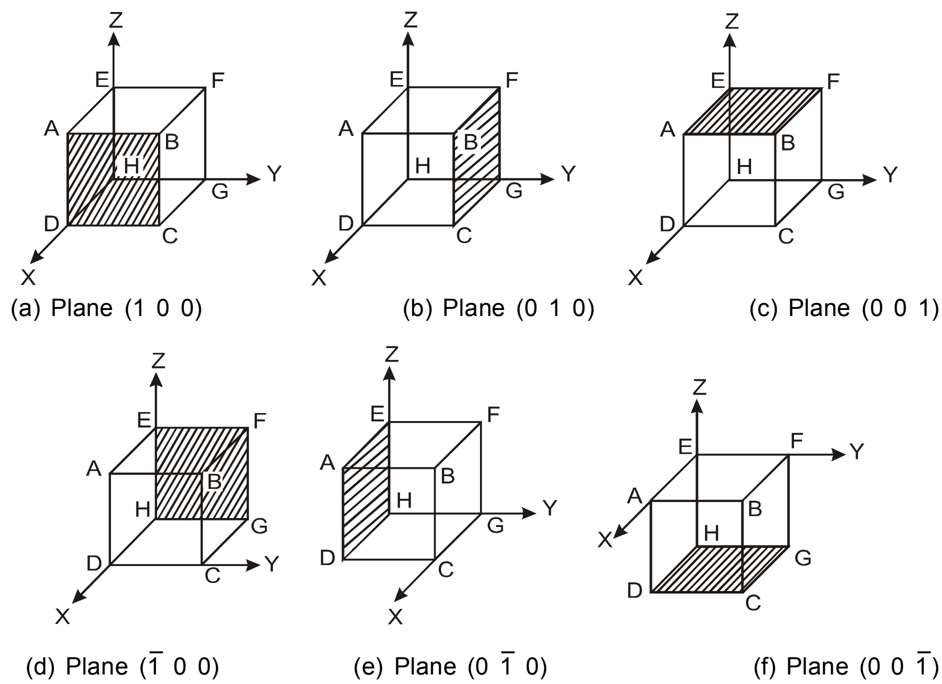


Fig. 3.6 *Crystal Planes*

2. For an intercept along the negative axis, the indices of the plane are represented by taking the reciprocals of the intercept and placing a bar (–) over the integer (intercept value).

The Miller indices for the Figures 3.7 (d, e and f) are $(\bar{1}\ 0\ 0)$, $(0\ \bar{1}\ 0)$ and $(0\ 0\ \bar{1})$ respectively. To draw these planes the points, D, G and E are taken as the origin respectively.

Common Planes in a Simple Cubic Structure

Even though there are a number of planes that can be drawn, the most common planes in a simple cubic structure are (1 0 0), (1 1 0) and (1 1 1).

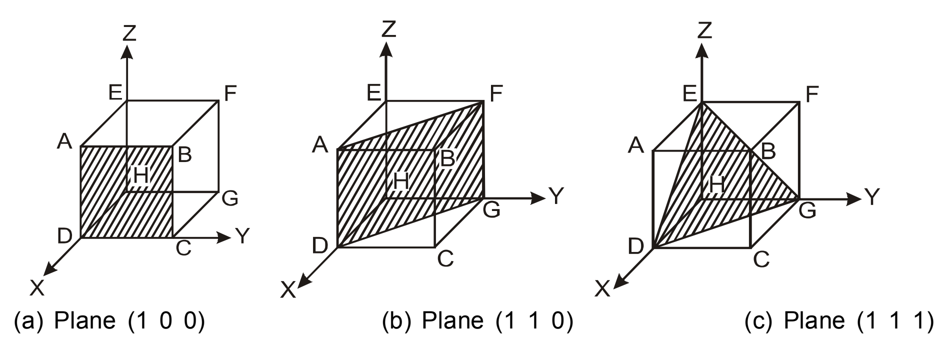


Fig. 3.7 *Common Planes*

NOTES

The three most important planes in a simple cubic structure are shown in Figure 3.7, and the way of drawing all the above planes are explained one by one.

Plane (100)

In this case h = 1, k = 0 and l = 0. The reciprocals of h, k and l are

$$\frac{1}{1}\frac{1}{0}\frac{1}{0} = 1\ \infty\ \infty$$

Now, sketch the plane with intercepts (1, ∞ , ∞) along the X, Y and Z axes, respectively, see Figure 3.8(a).

Plane (110)

In this case h = 1, k = 1 and l = 0. The reciprocals of h, k and l are

$$\frac{1}{1}\frac{1}{1}\frac{1}{0} = 1\ \ 1\ \ \infty$$

Now, sketch the plane with intercepts (1, 1, ∞) along the X, Y and Z axes, respectively, see Figure 3.8(b).

Plane (111)

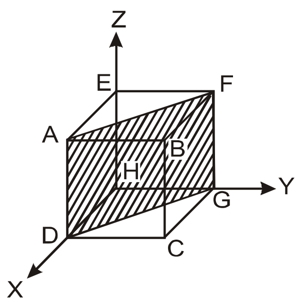
In this case h = 1, k = 1 and l = 1. The reciprocals of h, k and l are

$$\frac{1}{1}\frac{1}{1}\frac{1}{1} = 1\ 1\ 1$$

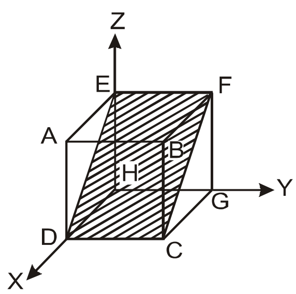
Now, sketch the plane with intercepts (1, 1, 1) along the X, Y and Z axes, respectively, see Figure 3.8(c).

Families of Planes

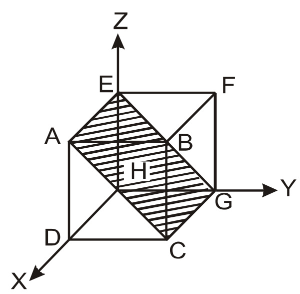
Depending on the crystal system, two or more planes may belong to the same family of planes.



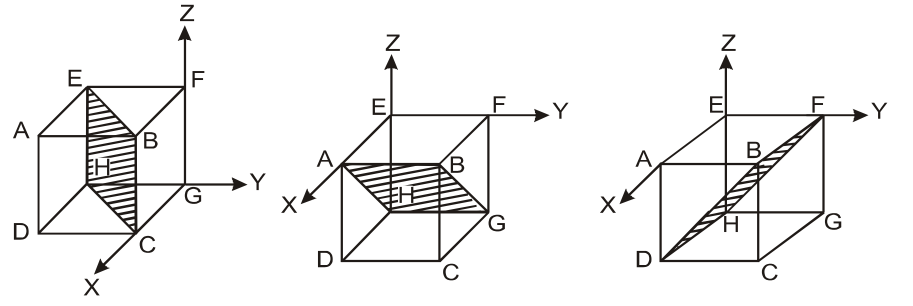
(a) Plane (1 1 0)



(b) Plane (1 0 1)



(c) Plane (0 1 1)



(d) Plane ($\bar{1}\ \bar{1}\ 0$) (e) Plane ($\bar{1}\ 0\ \bar{1}$) (f) Plane ($0\ \bar{1}\ \bar{1}$)

Fig. 3.8 *Crystal Planes*

For a cubic unit cell, we know that all the planes or six faces are of the same form. An example of multiple planes in a cubic system is shown in Figure 3.9. The following planes constitute a family of planes.

For a cubic unit cell, we know that all the planes or six faces are of the same form. An example of multiple planes in a cubic system is shown in Figure 3.9. The following planes constitute a family of planes.

$$\begin{bmatrix} (1\,0\,0),\ (0\,1\,0),\ (0\,0\,1) \\ \left(\bar{1}\,0\,0\right),\left(0\,\bar{1}\,0\right),\left(0\,0\,\bar{1}\right) \end{bmatrix} = \{1\,0\,0\}$$

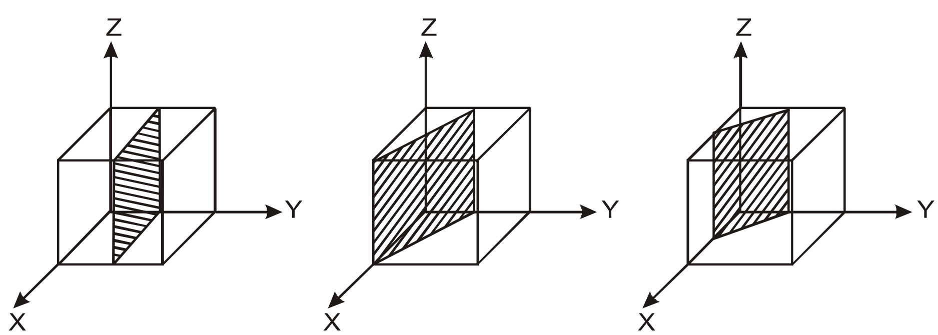
The collective notation for a family of planes is (hkl).

Each plane is identical except for the consequences of our arbitrary choice of axis labels and directions.

Similarly {1 1 1} family includes 8 planes and the {1 1 0} family includes 12 planes.

Example 3.1

Figure 3.9 shows the three crystal planes. Compute the Miller indices of the given planes.



(a) (b) (c)

Fig. 3.9

NOTES

Solution:

In Figure 3.10(a) the given plane is parallel to X and Z axes. Thus, its numerical intercepts on these two axes are infinity.

The numerical intercept on Y axis is 1/2 or 0.5. Thus, the numerical intercepts of the plane is (∞, 1/2, ∞).

∴ Miller indices of the plane is (0 2 0).

In Figure 3.10(b) the given plane is parallel to Z axis. Thus, its numerical intercept on the Z axis is infinity.

The numerical intercept on X axis is 1 and Y axis is 1/2. Thus, the numerical intercepts of the plane is (1, 1/2, ∞).

∴ Miller indices of the plane is (1 2 0).

In Figure 3.10(c) the given plane is parallel to Z axis. Thus, its numerical intercept on this Z axis is infinity.

The numerical intercept on X and Y axis is 1/2 and 1/2, respectively. Thus, the numerical intercepts of the plane is (1/2, 1/2, ∞).

∴ **Miller indices of the plane is (2 2 0).**

Example 3.2

Draw the following planes in a cubic structure: (1 1 2), (0 0 1), (1 0 1), (2 0 0) and (1 0 0).

Solution:

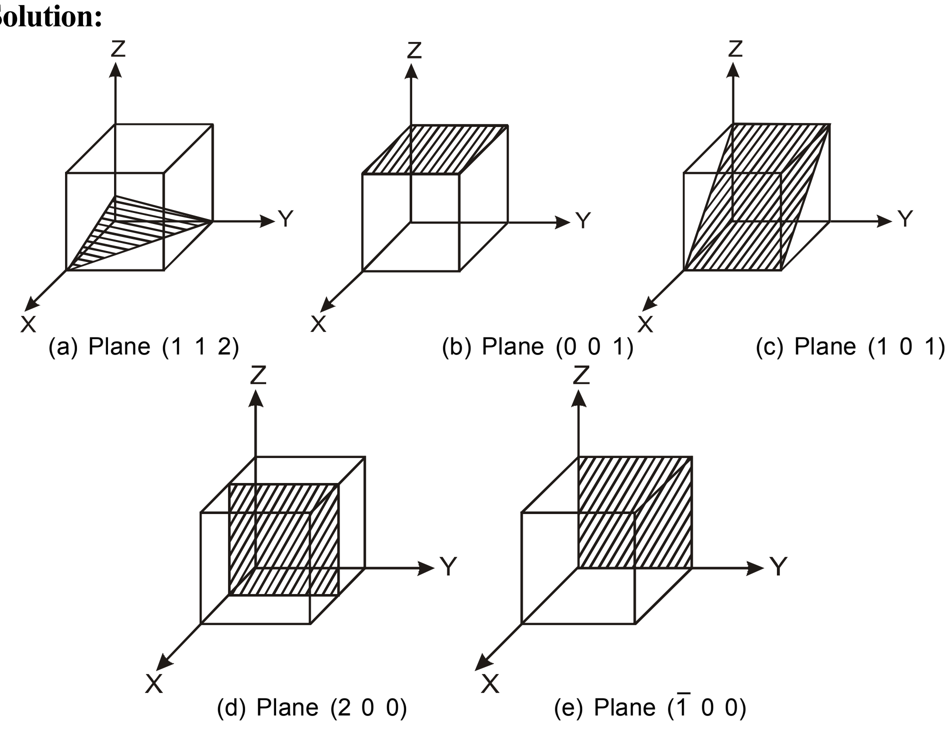


Fig. 3.10

NOTES

3.5 RECIPROCAL LATTICE

Procedure for Sketching the Plane from the Given Miller Indices

The following procedure is adopted for sketching any plane when its Miller indices are given.

As a first step, take the reciprocals of the given Miller indices. These reciprocals represent the intercepts in terms of the axial units along the X, Y and Z axes, respectively.

For example, let the Miller indices be (2 2 1). Therefore, its reciprocals of intercepts will be $\frac{1}{2}, \frac{1}{2}$ and $\frac{1}{1}$ or 0.5, 0.5 and 1, respectively.

Now sketch the plane with intercepts of 0.5, 0.5 and 1 along the X, Y and Z axes, respectively, as shown in Figure 3.11.

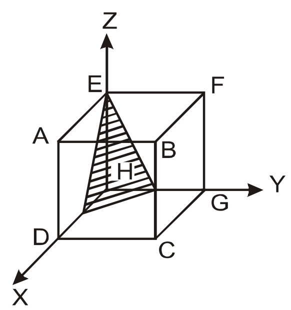


Fig. 3.11 *Plane (2 2 1)*

3.6 WIGNER-SEITZ CELLS

A special type of primitive-cells is known as the Wigner-Seitz cell. The Wigner-Seitz cell of a lattice point is constructed by the volume that occupies all the points in phase space closer to this particular lattice point as compared to others. It can be created as shown in the figure below:

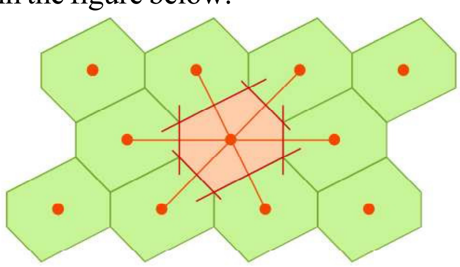


Fig. 3.12 *The 2D-Formation of a Wigner-Seitz Cell: Firstly, Choose Any Lattice Point and Draws Connecting Lines to its Neighboring Lattice Points. Afterward, Draw the Perpendicular Bisectors of these Lines. The Enclosed Area Formed by these Lines is the Wigner-Seitz Cell. It Forms a Repeated Unit Covering the Whole Structure with Any mismatch*

NOTES

Wigner and Seitz also showed that for the band structure of the crystal of an alkali metal like Na, there is no difference amongst the electron wave function of free atoms and nearly free model of the electron. Over most of a band, the energy may depend on the wave vector nearly as it depends on a free electron. However, the Bloch wave function will pile-up the charge on the positive ion cores as in the atomic wave function.

Construction of Wigner-Seitz Cells

The following steps need to be applied to form a Wigner-Seitz cell.

1. Choose any lattice site as the origin.
2. Draw vectors joining to all neighbouring lattice points to the origin.
3. Construct planes perpendicularly bisecting all the vectors.
4. The enclosed area formed by joining these planes is the Wigner-Seitz cell.

The Characteristics of Wigner-Seitz cell

1. Wigner-Seitz cells are identical in shape, size, and orientation. Besides, follows the translational symmetry of the lattice.
2. When stacked the Wigner-Seitz cells fill all space.
3. The Wigner-Seitz cells are polyhedron in shape.
4. The Wigner-Seitz cell demonstrates point symmetry among its lattice points.

A Wigner–Seitz cell is an example of a primitive cell, which is a unit cell containing exactly one lattice point. For any given lattice, there are an infinite number of possible primitive cells. However, there is only one Wigner–Seitz cell for any given lattice. It is the locus of points in space that are closer to that lattice point than to any of the other lattice points. The Wigner–Seitz cell, named after Eugene Wigner and Frederick Seitz, is a primitive cell which has been constructed by applying Voronoi decomposition to a crystal lattice. It is used in the study of crystalline materials in solid-state physics as well as in condensed matter physics.

The unique property of a crystal is that its atoms are arranged in a regular three-dimensional array called a lattice. All the properties attributed to crystalline materials stem from this highly ordered structure. Such a structure exhibits discrete translational symmetry. In order to model and study such a periodic system, one needs a mathematical "Handle" to describe the symmetry and hence draw conclusions about the material properties consequent to this symmetry. The Wigner–Seitz cell is a means to achieve this.

A Wigner–Seitz cell, like any primitive cell, is a fundamental domain for the discrete translation symmetry of the lattice. The primitive cell of the reciprocal lattice in momentum space is called the Brillouin zone.

NOTES

The Wigner–Seitz cell around a lattice point is defined as the locus of points in space that are closer to that lattice point than to any of the other lattice points. It can be shown mathematically that a Wigner–Seitz cell is a primitive cell. This implies that the cell spans the entire direct space without leaving any gaps or holes, a property known as tessellation. The Wigner–Seitz cell always has the same point symmetry as the underlying Bravais lattice. For example, the cube, truncated octahedron, and rhombic dodecahedron have point symmetry O_h, since the respective Bravais lattices used to generate them all belong to the cubic lattice system, which has O_h point symmetry.

In practice, the Wigner–Seitz cell itself is actually rarely used as a description of direct space, where the conventional unit cells are usually used instead. However, the same decomposition is extremely important when applied to reciprocal space. The Wigner–Seitz cell in the reciprocal space is called the Brillouin zone, which contains the information about whether a material will be a conductor, semiconductor or an insulator.

3.7 BONDING IN SOLIDS

Every solid (crystalline or amorphous) contains electrons. The important question is that "how the electrons respond when an electric field is applied to it?" That means "how electrical conductivity plays role for different solids?" We already know that the electrons in a crystalline solids are arranged in regular manner. These electrons in crystals are arranged in "Energy Bands" separated by regions in energy for which no wavelike electron orbitals exist. Such forbidden regions are called "*Energy Gaps* (E_g)" or "*Band Gap* (E_g)".

Let us consider two standing waves $\psi_+(x, t)$ and $\psi_-(x, t)$ pile up electrons at different regions, therefore the two standing waves have different potential energy. This is the origin of the "Band Gap" or "Energy Gap". In a constant potential (free electron theory), the energy of the electron as function of the wave vector $\vec{K}$ is given by

$$E = \frac{\hbar^2 K^2}{2m} \qquad ...(3.8)$$

Where $$K = \frac{2\pi}{\lambda} = \frac{P}{\hbar}$$

However, if we consider the motion of an electron in a periodic potential, we can say

(*i*) There exist allowed energy bands separated by forbidden regions; and

(*ii*) The functions $E(K)$ are periodic in $\vec{K}$.

The Figure (3.13) shows the plot of energy E with wave vector K (or wave number) for a free electron.

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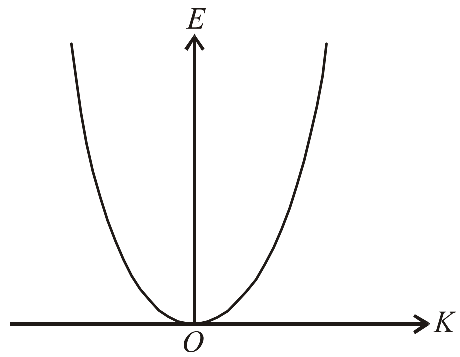


Fig. 3.13 *Energy (E) vs. Wave Vector (K) Graph for a Free Electron*

Figure (3.14) shows the plot of energy E with vector K (or wave number) in a monatomic lattice of lattice constant 'a'. Here, the energy gap (E_g) associated with the first Bragg's reflection at $K = \pm \pi/a$. Other forbidden gaps are found at $\pm n\pi/a$, where $n = 1, 2, 3,....$ etc.

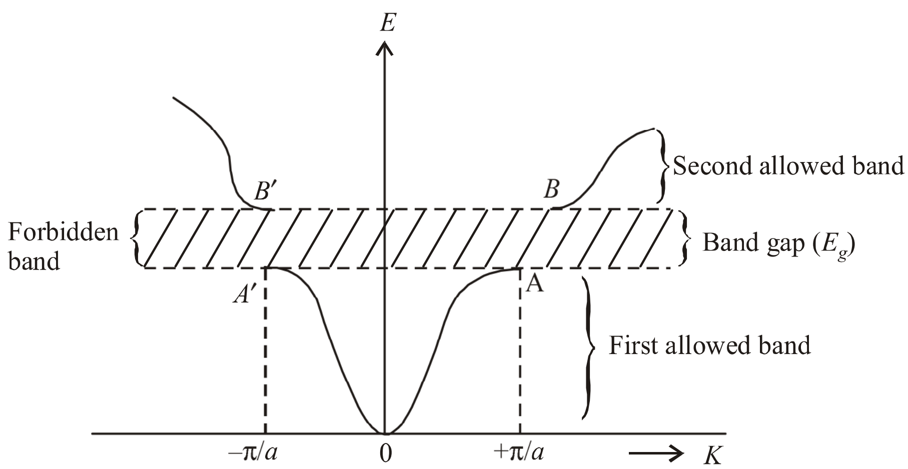


Fig. 3.14 *Energy (E) vs. Wave Vector (K) Graph for a Monatomic Lattice of Lattice Constant 'a'*

Check Your Progress

1. Explain the different types of lattices.
2. What is hexagonal close packed structure?
3. Define the Atomic Packing Factor (APF).
4. Illustrate the Miller indices.
5. Elaborate on the reciprocal lattice.
6. State the Wigner-Seitz cells.

3.8 ANSWERS TO CHECK YOUR PROGRESS QUESTIONS

NOTES

1. There are three types of lattices possible in this system depending on the positions of the lattice points in the unit cell- (i) Simple Cubic or Primitive (SC or P), (ii) Body Centered Cubic (BCC), and (iii) Face Centered Cubic (FCC).
2. In the hexagonal close packed structure, the unit cell contains one atom at each corner of the two hexagonal prisms (top and bottom), one atom each at the centre of the hexagonal faces and three more atoms within the body of the cell.
3. $$\text{APF} = \frac{\text{Number of atoms per unit cell} \times \text{Volume of one atom}}{\text{Volume of the unit cell}}$$
4. Miller introduced a set of three numbers to designate a plane in a crystal. This set of three numbers is known as Miller indices of the concerned plane. Thus, Miller indices may be defined as the reciprocal of the intercepts made by the plane along the three crystallographic axes which are reduced to smallest numbers.
5. Take the reciprocals of the given Miller indices. These reciprocals represent the intercepts in terms of the axial units along the X, Y and Z axes, respectively.
6. The Wigner–Seitz cell, named after Eugene Wigner and Frederick Seitz, is a primitive cell which has been constructed by applying Voronoi decomposition to a crystal lattice. It is used in the study of crystalline materials in solid-state physics as well as in condensed matter physics.

3.9 SUMMARY

- There are three types of lattices possible in this system depending on the positions of the lattice points in the unit cell- (i) Simple Cubic or Primitive (SC or P) , (ii) Body cantered cubic (BCC), and (iii) Face cantered cubic (FCC).
- In the hexagonal close packed structure, the unit cell contains one atom at each corner of the two hexagonal prisms (top and bottom), one atom each

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at the centre of the hexagonal faces and three more atoms within the body of the cell.

- Miller introduced a set of three numbers to designate a plane in a crystal. This set of three numbers is known as Miller indices of the concerned plane. Thus, Miller indices may be defined as the reciprocal of the intercepts made by the plane along the three crystallographic axes which are reduced to smallest numbers.
- Miller indices are the three smallest possible integers, which have the same ratio as the reciprocals of the intercepts of the plane concerned along the three axes.
- Take the reciprocals of the given Miller indices. These reciprocals represent the intercepts in terms of the axial units along the X, Y and Z axes, respectively.
- A Wigner–Seitz cell is an example of a primitive cell, which is a unit cell containing exactly one lattice point. For any given lattice, there are an infinite number of possible primitive cells.
- The Wigner–Seitz cell, named after Eugene Wigner and Frederick Seitz, is a primitive cell which has been constructed by applying Voronoi decomposition to a crystal lattice. It is used in the study of crystalline materials in solid-state physics as well as in condensed matter physics.
- A Wigner–Seitz cell, like any primitive cell, is a fundamental domain for the discrete translation symmetry of the lattice. The primitive cell of the reciprocal lattice in momentum space is called the Brillouin zone.

3.10 KEY WORDS

- **Types of Lattices:** There are three types of lattices possible in this system depending on the positions of the lattice points in the unit cell- (i) Simple Cubic or Primitive (SC or P) , (ii) Body cantered cubic (BCC), and (iii) Face cantered cubic (FCC).
- **Hexagonal close packed:** In the hexagonal close packed structure, the unit cell contains one atom at each corner of the two hexagonal prisms (top and bottom), one atom each at the centre of the hexagonal faces and three more atoms within the body of the cell.

- **Atomic packing factor (APF):**
- **Miller indices:** Miller indices may be defined as the reciprocal of the intercepts made by the plane along the three crystallographic axes which are reduced to smallest numbers.
- **Wigner-Seitz cells:** A Wigner–Seitz cell is an example of a primitive cell, which is a unit cell containing exactly one lattice point. For any given lattice, there are an infinite number of possible primitive cells.

3.11 SELF ASSESSMENT QUESTIONS AND EXERCISES

Short-Answer Questions

1. Define the different types of lattices.
2. Interpret the hexagonal close packed structure.
3. Explain the atomic packing factor (APF).
4. State the Miller indices.
5. Illustrate the reciprocal lattice.
6. Elaborate on the Wigner-Seitz cells.

Long-Answer Questions

1. Discuss briefly the different types of lattices: SC, BCC, and FCC with the help of examples.
2. Explain the Miller indices.
3. Illustrate the Reciprocal lattice. Give appropriate example.
4. Describe the Wigner-Seitz Cells.
5. Analyse the bonding in solids.

3.12 FURTHER READINGS

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BLOCK - II
LATTICE VIBRATIONS, BAND THEORY OF SOLIDS AND DIELECTRIC PROPERTIES OF MATERIALS

UNIT 4 LATTICE VIBRATIONS

Structure

4.0 Introduction
4.1 Objectives
4.2 Lattice Vibrations
4.3 Diatomic Lattices
4.4 Phonons
4.5 Answers to Check Your Progress Questions
4.6 Summary
4.7 Key Words
4.8 Self Assessment Questions and Exercises
4.9 Further Readings

4.0 INTRODUCTION

Lattice Vibration is the fluctuations of atoms in a solid with reference to the equilibrium position. Lattice vibrations can describe elastic properties, thermal properties, optical properties, and sound velocity of materials. In a crystal, the equilibrium positions form a regular lattice. The vibration of these neighbouring atoms is not independent of each other. A regular lattice with harmonic forces between atoms and normal modes of vibrations are called lattice waves. Lattice waves range from low frequencies to high frequencies on the order of 1,013 Hz or even higher.

Lattice vibrations can also relate with free electrons in a conducting solid which gives intensification to electrical resistance. Due to the connections between atoms, the displacement of one or more atoms from their equilibrium positions gives rise to a set of vibration waves propagating through the lattice. One such wave is shown in the figure to the right. The amplitude of the wave is given by the displacements of the atoms from their equilibrium positions. The wavelength λ is marked.

There is a minimum possible wavelength, given by twice the equilibrium separation a between atoms. Any wavelength shorter than this can be mapped onto a wavelength longer than $2a$, due to the periodicity of the lattice. This can be thought as one consequence of Nyquist–Shannon sampling theorem, the lattice points are viewed as the “Sampling Points” of a continuous wave.

Diatomic lattices played an important role in the elucidation of the concepts of element, atom, and molecule in the 19th century, because some of the most

common elements, such as hydrogen, oxygen, and nitrogen, occur as diatomic molecules. John Dalton's original atomic hypothesis assumed that all elements were monatomic and that the atoms in compounds would normally have the simplest atomic ratios with respect to one another.

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The study of phonons is an important part of condensed matter physics. They play a major role in many of the physical properties of condensed matter systems, such as thermal conductivity and electrical conductivity, as well as play a fundamental role in models of neutron scattering and related effects.

In this unit, you will study about the lattice vibrations, diatomic lattices, and phonons.

4.1 OBJECTIVES

After going through this unit, you will be able to:

- Comprehend the lattice vibrations
- Define the diatomic lattices
- Elaborate on the phonons

4.2 LATTICE VIBRATIONS

When a lattice is at its equilibrium position then each atom is directed exactly at its lattice site. Now suppose that an atom is displaced from its equilibrium position by an infinitesimal amount. It will tend to regain its equilibrium position, due to the restoring forces acting on it. This causes lattice vibrations. Numerous atoms move simultaneously, therefore, this has to be considered as the motion of the entire lattice.

Lattice vibrations can describe elastic properties, thermal properties, optical properties, and sound velocity of materials. Lattice Vibration is the fluctuations of atoms in a solid with reference to the equilibrium position.

In a crystal, the equilibrium positions form a regular lattice. The vibration of these neighbouring atoms is not independent of each other. A regular lattice with harmonic forces between atoms and normal modes of vibrations are called lattice waves. Lattice waves range from low frequencies to high frequencies on the order of 1,013 Hz or even higher.

Lattice vibrations can also relate with free electrons in a conducting solid which gives intensification to electrical resistance. Due to the connections between atoms, the displacement of one or more atoms from their equilibrium positions gives rise to a set of vibration waves propagating through the lattice. One such wave is shown in the figure to the right. The amplitude of the wave is given by the displacements of the atoms from their equilibrium positions. The wavelength λ is marked.

Due to the connections between atoms, the displacement of one or more atoms from their equilibrium positions gives rise to a set of vibration waves

propagating through the lattice. One such wave is shown in the figure to the right. The amplitude of the wave is given by the displacements of the atoms from their equilibrium positions. The wavelength λ is marked.

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There is a minimum possible wavelength, given by twice the equilibrium separation a between atoms. Any wavelength shorter than this can be mapped onto a wavelength longer than $2a$, due to the periodicity of the lattice. This can be thought as one consequence of Nyquist–Shannon sampling theorem, the lattice points are viewed as the "Sampling Points" of a continuous wave. Not every possible lattice vibration has a well-defined wavelength and frequency. However, the normal modes do possess well-defined wavelengths and frequencies.

4.3 DIATOMIC LATTICES

Consider a one-dimensional lattice with two non-equivalent atoms in a unit cell. The diatomic lattice show an important feature which is different from the monoatomic case. Figure 4.1 shows a diatomic lattice with the unit cell composed of two atoms of masses M_1 and M_2 with the distance between two neighbouring atoms a.

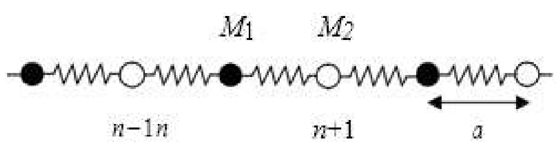


Fig. 4.1 *Diatomic Lattice with the Unit Cell*

We can evaluate the motion of this lattice in a similar way as for monoatomic lattice. However, in this case because we have two different types of atoms, we should write two equations of motion:

$$M_1 \frac{d^2 u_n}{dt^2} = -C(2u_n - u_{n+1} - u_{n-1}) \quad ...4.1$$

$$M_2 \frac{d^2 u_{n+1}}{dt^2} = -C(2u_{n+1} - u_{n+2} - u_n) \quad ... 4.2$$

In analogy with the monoatomic lattice we are looking for the solution in the form of traveling mode for the two atoms:

$$\begin{bmatrix} u_n \\ u_{n+1} \end{bmatrix} = \begin{bmatrix} A_1 e^{iqna} \\ A_2 e^{iq(n+1)a} \end{bmatrix} e^{-i\omega t}, \quad ..4.3$$

Which is written in the obvious matrix form. Substituting this solution to Equation 4.2, we get

$$\begin{bmatrix} 2C - M_1\omega^2 & -2C\cos qa \\ -2C\cos qa & 2C - M_2\omega^2 \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = 0 . \qquad ...4.4$$

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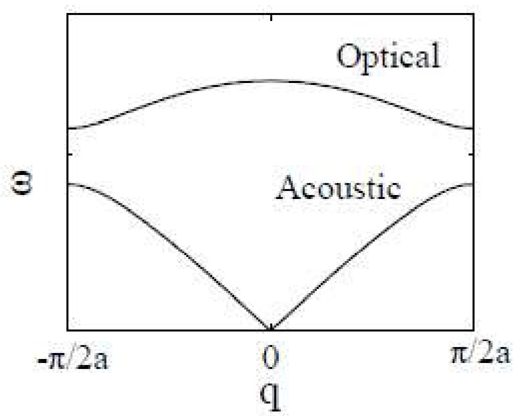
This is a system of linear homogeneous equations for the unknowns A_1 and A_2. A nontrivial solution exists only if the determinant of the matrix is zero. This leads to the secular equation

$$(2C - M_1\omega^2)(2C - M_2\omega^2) - 4C^2\cos^2 qa = 0 . \qquad ...\ 4.5$$

This is a quadratic equation, which can be readily solved:

$$\omega^2 = C\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4\sin^2 qa}{M_1 M_2}} . \qquad ...\ 4.6$$

Depending on sign in this formula there are two different solutions corresponding to two different dispersion curves, as is shown in below figure.



The lower curve is called the acoustic branch, while the upper curve is called the optical branch.

4.4 PHONONS

In condensed matter physics, a phonon is a collective excitation in a periodic, elastic arrangement of atoms or molecules in condensed matter, specifically in solids and some liquids. Often referred to as a quasi-particle, it is an excited state in the quantum mechanical quantization of the modes of vibrations for elastic structures of interacting particles.

Phonons can be thought of as quantized sound waves, similar to photons as quantized light waves. The concept of phonons was introduced in 1932 by Soviet physicist Igor Tamm.

NOTES

The study of phonons is an important part of condensed matter physics. They play a major role in many of the physical properties of condensed matter systems, such as thermal conductivity and electrical conductivity, as well as play a fundamental role in models of neutron scattering and related effects.

A phonon is the quantum mechanical description of an elementary vibrational motion in which a lattice of atoms or molecules uniformly oscillates at a single frequency. While normal modes are wave-like phenomena in classical mechanics, phonons have particle-like properties too, in a way related to the wave–particle duality of quantum mechanics.

Three important properties of phonons may be deduced from this technique. First, phonons are bosons, since any number of identical excitations can be created by repeated application of the creation operator $b_k^{\dagger}$. Second, each phonon is a "Collective Mode" caused by the motion of every atom in the lattice. This may be seen from the fact that the creation and annihilation operators, defined here in momentum space, contains sums over the position and momentum operators of every atom when written in position space. Finally, using the position–position correlation function, it can be shown that phonons act as waves of lattice displacement.

Recent research has shown that phonons may have a non-negligible mass and be affected by gravity just as standard particles are. In particular, phonons are predicted to have a kind of negative mass and negative gravity. This can be explained by how phonons are known to travel faster in denser materials. Because the part of a material pointing towards a gravitational source is closer to the object, it becomes denser on that end. From this, it is predicted that phonons would deflect away as it detects the difference in densities, exhibiting the qualities of a negative gravitational field. Although the effect would be too small to measure, it is possible that future equipment could lead to successful results.

Phonons have also been predicted to play a key role in superconductivity in materials and the prediction of superconductive compounds. In 2019, researchers were able to isolate individual phonons without destroying them for the first time.

A lattice vibration carries quantized energy. The quantum of that energy is called a phonon, similar to the photon in electromagnetism. Phonons are specifically relevant for the behaviour of heat and sound transfer in the crystal. The atoms are uniformly arranged in a crystal. The atoms in a crystal can oscillate at particular frequencies when heated. The bonds between the individual atoms can be considered as elastic springs. When one atom of this entangled chain of atoms is pulled or pushed, a wave (or phonon) originates in the crystal as it happens in a rope.

Generally, most of the crystals are filled with a chaotic mixture of phonons comprising different frequencies and propagating in different directions. All waves superimpose each other and form a sea of several phonons.

Phonons are not exactly equivalent to photons, the quantized energy particles of electromagnetic radiation. The photons of different wavelengths majorly don't interact with each other. Whereas, the different phonons can interact and add up when they bump into each other and produce a changed wavelength. Such a property makes them random and hard to control.

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The energy of a phonon behaves similar to the photons of a given energy, defined by their frequency, can impart energy into a system only in integer multiples of the basic quanta. Moreover, the heat transfer phenomenon in solids can also be imagined in terms of the propagation of phonons.

In electronic devices, such as computer chips, the process of heat dissipation is quite important to keep components work fine. The ways are designed to control the motion of phonons to get chips cool faster and perform better. On the other hand, some other methods are also designed where the system is allowed to transmit electricity but block heat for thermoelectric devices.

Phonon Momentum

It seems hard to believe that how a wave can carry a momentum but when a phonon interacts with elementary particles such as electron, proton, or neutrons, it seems like it carried a momentum of $hk/2\pi$ (where k is the wave vector). A phonon does not carry any physical momentum. The reason behind this is that a phonon coordinate (except for $k = 0$) includes relative coordinates of the atoms. In a hydrogen molecule (H_2), the internuclear vibrational coordinate $r_1 - r_2$ is a relative coordinate and it does not carry linear momentum. The center of mass coordinate agrees to the uniform mode for $k = 0$ and then it can carry a linear momentum. In crystals, wave vector selection rules guide the allowed transitions between different quantum states. The elastic scattering of an x-ray photon by a crystal is instructed by the wave vector selection rule

$$k' = k + G \qquad (4.7)$$

Where G is a vector in the phase space of reciprocal lattice, k is the wave vector of the incident photon, and k' is the wave vector of the scattered photon. In the process of reflection, the crystal as a whole will recoil with the momentum — hG, but this uniform mode of momentum is considered explicitly very rarely.

Equation (4.7) is an example of the rule that the total wave vector of the interacting waves is conserved in a periodic lattice, with the possible addition of a reciprocal lattice vector G. The true momentum of the whole system always is severely conserved. If the scattering of the photon is inelastic, along with the creation of a phonon of wave vector K, then the wave vector selection rule becomes

$$k' + K = k + G\,, \qquad (4.8)$$

If a phonon K is absorbed in this process, we have instead of the relation

$$k' = k + K + G\,. \qquad (4.9)$$

Relations (4.8) and (4.9) are the natural extensions of (4.7).

Check Your Progress

1. Explain the lattice vibrations.
2. What do you understand by the diatomic lattices?
3. Elaborate on the phonons.

4.5 ANSWERS TO CHECK YOUR PROGRESS QUESTIONS

NOTES

1. Lattice vibrations can describe elastic properties, thermal properties, optical properties, and sound velocity of materials. Lattice Vibration is the fluctuations of atoms in a solid with reference to the equilibrium position.
2. Consider a one-dimensional lattice with two non-equivalent atoms in a unit cell. The diatomic lattice show an important feature which is different from the monoatomic case.
3. In condensed matter physics, a phonon is a collective excitation in a periodic, elastic arrangement of atoms or molecules in condensed matter, specifically in solids and some liquids.

4.6 SUMMARY

- Lattice vibrations can describe elastic properties, thermal properties, optical properties, and sound velocity of materials. Lattice Vibration is the fluctuations of atoms in a solid with reference to the equilibrium position.
- Lattice vibrations can also relate with free electrons in a conducting solid which gives intensification to electrical resistance. Due to the connections between atoms, the displacement of one or more atoms from their equilibrium positions gives rise to a set of vibration waves propagating through the lattice.
- Consider a one-dimensional lattice with two non-equivalent atoms in a unit cell. The diatomic lattice show an important feature which is different from the monoatomic case.
- In condensed matter physics, a phonon is a collective excitation in a periodic, elastic arrangement of atoms or molecules in condensed matter, specifically in solids and some liquids.
- Phonons can be thought of as quantized sound waves, similar to photons as quantized light waves. The concept of phonons was introduced in 1932 by Soviet physicist Igor Tamm.
- A phonon is the quantum mechanical description of an elementary vibrational motion in which a lattice of atoms or molecules uniformly oscillates at a single frequency.
- Phonons have also been predicted to play a key role in superconductivity in materials and the prediction of superconductive compounds. In 2019, researchers were able to isolate individual phonons without destroying them for the first time.

4.7 KEY WORDS

NOTES

- **Lattice vibrations:** Lattice Vibration is the fluctuations of atoms in a solid with reference to the equilibrium position.
- **Diatomic lattices:** Consider a one-dimensional lattice with two non-equivalent atoms in a unit cell. The diatomic lattice show an important feature which is different from the monoatomic case.
- **Phonons:** A phonon is a collective excitation in a periodic, elastic arrangement of atoms or molecules in condensed matter, specifically in solids and some liquids.

4.8 SELF ASSESSMENT QUESTIONS AND EXERCISES

Short-Answer Questions

1. Define the lattice vibrations.
2. Elaborate on the diatomic lattices.
3. Explain the term phonons.

Long-Answer Questions

1. Briefly describe the lattice vibrations with the help of examples.
2. Explain the diatomic lattices. Give appropriate examples.
3. Discuss briefly about the phonons.

4.9 FURTHER READINGS

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UNIT 5 FREE ELECTRON FERMI GAS

NOTES

Structure

5.0 Introduction
5.1 Objectives
5.2 Electrical Properties of Metals
5.3 Free Electron Gas on Three Dimensions
5.4 Fermi Energy
5.5 Hall Effect
5.6 Answers to Check Your Progress Questions
5.7 Summary
5.8 Key Words
5.9 Self Assessment Questions and Exercises
5.10 Further Readings

5.0 INTRODUCTION

The main assumption of the free electron model to describe the delocalized electrons in a metal can be derived from the Fermi gas. Since interactions are neglected due to screening effect, the problem of treating the equilibrium properties and dynamics of an ideal Fermi gas reduces to the study of the behaviour of single independent particles. In these systems the Fermi temperature is generally many thousands of kelvins, so in human applications the electron gas can be considered degenerate. The maximum energy of the fermions at zero temperature is called the Fermi energy. The Fermi energy surface in reciprocal space is known as the Fermi surface.

The nearly free electron model adapts the Fermi gas model to consider the crystal structure of metals and semiconductors, where electrons in a crystal lattice are substituted by Bloch electrons with a corresponding crystal momentum. As such, periodic systems are still relatively tractable and the model forms the starting point for more advanced theories that deal with interactions, for example using the perturbation theory.

A free Fermi gas is a physical model assuming a collection of non-interacting fermions in a constant potential well. Fermions are elementary or composite particles with half-integer spin, thus follow Fermi-Dirac statistics. The equivalent model for integer spin particles is called the Bose gas (an ensemble of non-interacting bosons). At low enough particle number density and high temperature, both the Fermi gas and the Bose gas behave like a classical ideal gas.

The total energy of the Fermi gas at absolute zero is larger than the sum of the single-particle ground states because the Pauli principle implies a sort of

interaction or pressure that keeps fermions separated and moving. For this reason, the pressure of a Fermi gas is non-zero even at zero temperature, in contrast to that of a classical ideal gas.

In this unit, you will study about the electrical properties of metals, the free electron gas in three dimensions, the Fermi energy, and the Hall effect.

5.1 OBJECTIVES

After going through this unit, you will be able to:

- Analyse the electrical properties of metals
- Explain the free electron gas in three dimensions
- Understand the Fermi energy
- Define the Hall effect

5.2 ELECTRICAL PROPERTIES OF METALS

The outstanding properties or characteristics of metals are listed below:

1. Metals have high electrical and thermal conductivities.
2. In the steady state, ohm's law is obeyed, i.e., $I \propto^{al} E$, which states that, the current in the steady state is proportional to the electric field.
3. Resistivity above Debye's temperature is proportional to the absolute temperature, i.e., $\rho \propto^{al} T$.
4. At low temperatures the resistivity of metal is proportional to the fifth power of absolute temperature, i.e., $\rho \propto^{al} T^5$.
5. For most metals, resistivity is inversely proportional to the pressure, i.e., $\rho \propto^{al} \frac{1}{P}$.
6. Above Debye's temperature, the ratio of thermal and electrical conductivities is directly proportional to the absolute temperature, and is known as Wiedemann-Franz law.

   i.e., $\frac{K}{\sigma} \propto^{al} T$ where K is the thermal conductivity and σ is the electrical conductivity.
7. At absolute zero, the resistivity tend zero, i.e., the specimen exhibits the phenomenon of superconductivity.
8. The conductivity of the specimen varies in the presence of magnetic field. This effect is called as magneto resistance effect.

Basic Terminologies in Electrical Conductivity

It is necessary to learn about the related terminologies in electrical conductivity, before we go for its derivation.

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Ohm's Law

When an electric current flows through a material, the magnitude of the current flowing through the material is given by ohm's law.

$$I = \frac{V}{R} \quad ...(5.1)$$

where I is the current in **ampere**, R is the resistance to the current flow in **ohm** and V is the voltage in **volt**. This law is applicable to most but not all materials.

Resistance (R)

The resistance R, is a geometry (size, shape and property) dependent factor of the material used.

$$R \propto^{al} \frac{l}{A}$$

or $$R = \frac{\rho l}{A} = \frac{l}{\sigma A} \quad ...(5.2)$$

where l is the length of the specimen in **m**, A is the area of cross section of the specimen in **m^2**, ρ is the electrical resistivity in **ohm-meter** and σ is the reciprocal of resistivity ρ called electrical conductivity. The unit of electrical conductivity is **ohm^{-1}– m^{-1}** or **mho – m^{-1}**. The **unit mho** is also called as **siemens S**.

Current Density (J)

Current density is defined as the current per unit area of crosssection of an imaginary plane held normal to the direction of flow of current in a current carrying conductor.

If I is the current and A is the area of cross-section, then current density is given by

$$J = \frac{I}{A} \quad ...(5.3)$$

Its unit is A/m^2.

Electric Field (E)

The electric field E, of a conductor of uniform cross section is defined as the potential drop (voltage) V per unit length.

i.e., $$E = \frac{V}{l} \quad ...(5.4)$$

Its unit is Vm^{-1}.

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Electrical Conductivity (σ)

A second form of ohm's law can be obtained by combining Equations (5.5) and (5.6)

From Equation (5.5) $V = IR$

From Equation (5.6) $R = \dfrac{l}{\sigma A}$

$$\therefore \quad V = \frac{Il}{\sigma A}$$

or $$\frac{I}{A} = \sigma \frac{V}{l}$$

or $$J = \sigma E \qquad \left[\because \frac{I}{A} = J \text{ and } \frac{V}{l} = E\right] \qquad ...[5.5]$$

$$\therefore \quad \sigma = \frac{J}{E}. \qquad ..[5.6]$$

Thus electrical conductivity can be defined as, the rate of charge flow across a unit area per unit potential gradient within a conductor.

The above Equation (5.5) is also a representation of ohm's law and can be verified, by substituting for σ and E.

From Equation (5.6) $J = \sigma E$

$$\therefore \quad \frac{I}{A} = \frac{1}{\rho}\frac{V}{l}$$

$$I = \frac{A}{\rho l} V$$

or $$I = \frac{1}{R}.V \qquad \left[\because R = \frac{\rho l}{A}\right]$$

$$\therefore \quad IR = V$$

Hence, Ohm's law is derived.

Relation between Current Density J, Drift Velocity v_d and Mobility m

The current density J can also be defined as follows:

If n is the number of charge carriers per unit volume (also called carrier density) in a conductor of length *l* with cross sectional area A then, the current flow through the conductor is given by

$$I = \frac{\text{Total charge}}{\text{Time}}$$

$$= \frac{neAl}{t} = n\, e\, A\, v_d$$

...[5.7]

where $V_d = \frac{l}{t}$ *is called the drift velocity. It is the average velocity gained by the charge carriers in the presence of an electric field.*

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But, we know $$J = \frac{I}{A}$$

∴ Using Equation (5.7), J can be written as

$$J = \frac{neAv_d}{A} = n\ e\ v_d$$

∴ $$J = nev_d \quad ...(5.8)$$

But J is also equal to σE. Therefore Equation (5.8) becomes,

$$\sigma\ E = nev_d$$

or $$\sigma = ne\frac{v_d}{E}$$

Hence, $$\sigma = n\ e\ \mu \quad ...(5.9)$$

where $\frac{v_d}{E} = \mu$ is called the mobility of the charge carrier. *It is defined as the drift velocity per unit electric field. Its unit is* $m^2\ V^{-1}s^{-1}$. In the case of metals, this μ is the mobility of electrons. Hence, σ = neμ. This expression gives the relation between conductivity and mobility. Thus, the electrical conductivity of materials can be controlled by controlling the number of charge carriers per unit volume or by controlling the mobility of charge carriers.

The mobility is important in metals. But, in semiconductors and insulators, the number of charge carrier n is important.

In semiconductors, since electrons and holes are both involved in conduction, the expression for conductivity becomes

$$\sigma = n_e e\mu_e + n_h e\mu_h \quad ...(5.10)$$

Where n_e is the density of electrons.

n_h is the density of holes.

μ_e is the mobility of electrons.

μ_h is the mobility of holes.

Electron Theory of Metals

The study of valence electrons present in a band, which controls the various properties of metals is known as electron theory of metals.

The electron theory of metals is classified into the following three types.

1. Classical free electron theory or Drude-Lorentz theory.
2. Quantum free electron theory or Sommerfeld theory.
3. Zone theory or Band theory of solids.

Classical Free Electron Theory of Metals

This theory was developed by Drude and Lorentz. Eventhough it is a macroscopic theory it successfully explained most of the properties of metals.

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In this theory, the free electrons in a metal are treated like molecules in a gas and Maxwell-Boltzmann statistics is applied.

The main assumptions or postulates of this theory are:

1. A metal is composed of positive metal ion fixed in the lattice.
2. All the valence electrons are free to move among the ionic array. Such freely moving electrons contribute towards conduction (electrical and thermal) in metals.
3. There are a large number of free electrons in a metal and they move about the whole volume like the molecules of a gas.
4. The free electrons collide with the positive ions in the lattice and also among themselves. All the collisions are elastic, i.e., there is no loss of energy.
5. The electrostatic force of attraction between the free electrons and the metallic ions are neglected, i.e., the total energy of free electron is equal to its kinetic energy.
6. All the free electrons in metal have wide range of energies and velocities.
7. In the absence of electric field, the random motion of free electron is equally probable in all directions. So, the net current flow is zero.
8. When an electric field is applied as shown in Figure 5.1 the electrons gain a velocity called drift velocity V_d and moves in opposite direction to the field resulting in a current flow in the direction of field.

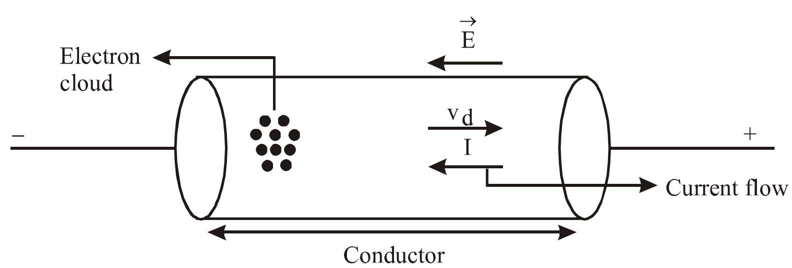


Fig. 5.1 *Conduction of Electrons in a Metal*

Thus, drift velocity is the average velocity acquired by an electron on applying an electric field.

Relaxation Time (τ)

Definition - 1 : *It is defined as the time required for the drift velocity to reduce to (1/e) times of its initial value, just when the field is switched off.*

Definition - 2 : *It is defined as the time taken by the free electron to reach its equilibrium position from its disturbed position just when the field is switched off.*

Mean Collision Time (τ_c)

The average time between two consecutive collisions of an electron with the lattice points is called collision time.

Mean Free Path (λ)

It is the average distance travelled by the conduction electron between successive collisions with the lattice ions.

In the following sections, based on classical free electron theory, expression for electrical conductivity, thermal conductivity and Wiedemann-Franz law is derived.

Note:

- **Bound Electrons –** All the valence electrons in an isolated atom bound to their parent nuclei are called as bound electrons.
- **Free Electrons –** In a solid, due to the boundaries of neighbouring atoms overlap each other, the valence electrons find continuity from atom to atom; and thus, can move easily throughout the solid. All such valence electrons of its constituent atoms in a solid are called as free electrons.

  The movements of the free electrons are confined to regions within the boundaries of the solid.
- **Difference between Ordinary Gas and the Free Electron Gas**

  The molecules of ordinary gas are neutral. But, the free electron gas is charged.

  The density of molecules is smaller than the density of free electrons.

Electrical Conductivity (S)

The electrical conductivity σ is defined as the rate of charge flow across a unit area in a conductor per unit potential (voltage) gradient.

i.e., $$\sigma = \frac{J}{E} \qquad ...(5.11)$$

Its unit is **mho–m^{-1} or Ω^{-1} m^{-1}.**

Expression for Electrical Conductivity

Electrical conductivity of a conductor is the property by which it allows the flow of electric current. *In a metal, the valence electrons are not attached to the individual atoms and are free to move about within the lattice. Hence, the valence electrons are also called free electrons or conduction electrons.*

In the absence of an electric field, the motion of the free electrons are completely random like those of the molecules of a gas in a container. But, when an electric field is applied to a metal, the electrons modify their random motion

NOTES

in such a way that, they drift slowly in the opposite direction to that of the applied field with an average velocity called the drift velocity v_d.

When an electric field E is applied, the free electrons in a metal experiences a force eE. Due to this force, the acceleration "*a*" gained by the electron is,

$$F = eE$$

$$ma = eE \qquad [\because F = ma]$$

or
$$a = \frac{eE}{m} \qquad ...(5.12)$$

Consider an electron that has just collided with an ion core. The collision momentarily destroys the tendency to drift and the electron will have truly random direction after this collision. In the next collision, the electrons velocity would have changed, to an average value v_d given by,

$$v_d = a\tau \qquad ...(5.13)$$

Where τ is called the mean free time.

Substituting Equation (5.12) in (5.13), we get

$$v_d = \frac{eE\tau}{m} \qquad ...(5.14)$$

The current density is given by

$$J = nev_d \qquad ...(5.15)$$

where, n is the number of free electrons per unit volume.

Hence, substituting Equation (5.14) in (5.15), we get

$$J = ne \times \frac{eE\tau}{m}$$

$\therefore$
$$J = \frac{ne^2\tau}{m}.E \qquad ...(5.16)$$

But, J is also expressed as,

$$J = \sigma E \qquad ...(5.17)$$

Therefore, substituting for J in Equation (5.16) from Equation (5.17),

$$\sigma E = \frac{ne^2\tau}{m}.E$$

or
$$\sigma = \frac{ne^2\tau}{m} \qquad ...(5.18)$$

Thus, the above expression relates the electrical conductivity to the number of free electrons per unit volume.

Expression for s in Terms of k_BT

The mean free time τ in terms of mean free path λ and average thermal velocity v is given by,

$$\tau = \frac{\lambda}{v} \qquad ...(5.19)$$

The kinetic energy of an electron based on kinetic theory is given by

NOTES

$$\frac{1}{2}mv^2 = \frac{3}{2}k_BT$$

(where k_B is the Boltzmann constant)

or $$m = \frac{3k_BT}{v^2} \qquad ...(5.20)$$

Substituting Equation (5.20) for m and Equation (5.19) for τ in Equation (5.18)

$$\sigma = \frac{ne^2\tau}{\frac{3k_BT}{v^2}} = \frac{ne^2\lambda}{3k_BT.v}.v^2$$

∴ $$\sigma = \frac{ne^2\lambda v}{3k_BT} \qquad ...(5.21)$$

Thus, from the above expression of σ it is observed that, the electrical conductivity of a metal decreases with increase of temperature.

Note:
- For an isotropic material the mean collision time τ_c is equal to the relaxation time τ. i.e., $\tau_c = \tau$.
- **Determination of Density of Electrons**

  (Determination of number of electrons / unit volume in terms of Avagadro's number).

  The density of Free Electrons or the number of free electrons/unit volume is n = Number of Free Electrons / Atom × Number of Atoms/Unit Volume

  To Evaluate Number of Atoms / Unit Volume

  In general, the volume occupied by 1 kg of a material is = $\frac{1}{D}$ **m³**

  $$\left[\because \text{Volume} = \frac{\text{Mass}}{\text{Density}}\right]$$

  Where D, is the density of the material.

  Therefore, volume occupied by a material of mass, equal to its atomic weight in kg

  $$= \frac{\text{Atomic Weight}}{D}\ \mathbf{m^3} \qquad ...(5.22)$$

  But we know, the number of atoms in a material of mass equal to its atomic weight in kg = N_A (The Avagadro number expressed per k mole).

  ...(5.23)

NOTES

Therefore, number of atoms in a volume of $\left[\dfrac{\text{Atomic Weight}}{D}\right] = N_A$

Hence, number of atoms / unit volume of the material = $\dfrac{N_A \times D}{\text{Atomic Weight}}$ ...(5.24)

Hence, substituting Equation (5.24) in (5.22) we get,

The density of electrons or the number of electrons / unit volume n =

Number of Free Electrons / Atom × $\mathbf{\dfrac{N_A \times D}{\text{Atomic Weight}}}$ $\mathbf{m^{-3}}$**.**

Example 5.1

A conductor has electron concentration of 5.9×10^{28} m^{-3}. What current density in the conductor corresponds to a drift velocity of 0.625 ms^{-1}? Calculate the mobility of the charge carriers. Given $\sigma = 6.22 \times 10^7\ \Omega^{-1}\ m^{-1}$.

Solution:

Given, $n = 5.9 \times 10^{28}\ m^{-3}$; $v_d = 0.625\ ms^{-1}$; $\sigma = 6.22 \times 10^7\ \Omega^{-1}\ m^{-1}$; J = ?; μ = ?

Formula

$$J = nev_d$$

$$= 5.9 \times 10^{28} \times 1.6 \times 10^{-19} \times 0.625$$

$$\therefore \quad \mathbf{J = 5.9 \times 10^9\ \ Am^{-2}}$$

We know

$$\sigma = ne\mu$$

$$\therefore \quad \mu = \frac{\sigma}{ne} = \frac{6.22 \times 10^7}{5.9 \times 10^{28} \times 1.6 \times 10^{-19}}$$

$$\mathbf{\mu = 6.588 \times 10^{-3}\ \ m^2\ V^{-1} s^{-1}.}$$

Example 5.2

Find the drift velocity of the free electrons in a copper wire whose cross-sectional area is A = 1.05 mm^2 when the wire carries a current of 1 A. Assume that, each copper atom contributes one electron to the electron gas. [Given density of free electrons in copper = 8.5×10^{28} m^{-3}].

Solution:

Given, $n = 8.5 \times 10^{28}\ m^{-3}$; $A = 1.05\ mm^2 = 1.05 \times 10^{-6}\ m^2$; I = 1A.

Formula

$$J = nev_d$$

$$\therefore \quad v_d = \frac{J}{ne} = \frac{I}{Ane}$$

$$\left[\because J = \frac{I}{A}\right]$$

$$v_d = \frac{1}{1.05\times10^{-6}\times8.5\times10^{28}\times1.6\times10^{-19}}$$

$$\mathbf{v_d = 7.002 \times 10^{-5}\ ms^{-1}.}$$

NOTES

Example 5.3

Calculate the drift velocity of the free electrons [with a mobility of $3.5 \times 10^{-3}\ m^2\ V^{-1}\ s^{-1}$] in copper for an elactric field strength of 0.5 V/m.

Solution:

Given, $\mu = 3.5 \times 10^{-3}\ m^2\ V^{-1}\ s^{-1}$; $E = 0.5\ Vm^{-1}$; $V_d = ?$;

Formula

$$v_d = \mu E$$

$$v_d = 3.5 \times 10^{-3} \times 0.5$$

$$\mathbf{v_d = 1.75 \times 10^{-3}\ ms^{-1}.}$$

Example 5.4

For a metal having 6.5×10^{28} conduction electrons per m^3, find the relaxation time of the conduction electrons if the metal resistivity is $1.435 \times 10^{-8}\ \Omega$–m.

Solution:

Given, $n = 6.5 \times 10^{28}\ m^{-3}$; $\rho = 1.435 \times 10^{-8}\ \Omega - m$; $\tau = ?$

Formula

$$\sigma = \frac{ne^2\tau}{m}$$

$$\therefore \qquad \tau = \frac{m\sigma}{ne^2} = \frac{m}{\rho ne^2}$$

$$\left[\because \sigma = \frac{1}{\rho}\right]$$

$$\therefore \qquad \tau = \frac{9.11\times10^{-31}}{1.435\times10^{-8}\times6.5\times10^{28}\times(1.6\times10^{-19})^2}$$

$$\boldsymbol{\tau = 3.815 \times 10^{-14}\ s.}$$

Example 5.5

Calculate the mean free path between collisions of the free electrons in copper at 20°C. The resistivity of copper at 20°C is $1.72 \times 10^{-8}\ \Omega m$ and density of free electrons is $8.48 \times 10^{+28}\ m^{-3}$.

Solution:

Given, $\rho = 1.72 \times 10^{-8}\ \Omega m$; T = 20°C = 293 K; $n = 8.48 \times 10^{+28}\ m^{-3}$; $\lambda = ?$

Formula

$$\sigma = \frac{ne^2\tau}{m}$$

NOTES

$$\therefore \quad \tau = \frac{m\sigma}{ne^2}$$

$$\tau = \frac{m}{\rho ne^2} = \frac{9.11\times10^{-31}}{1.72\times10^{-8}\times8.48\times10^{+28}\times(1.6\times10^{-19})^2}$$

$$\boldsymbol{\tau = 2.439 \times 10^{-14}} \textbf{ sec.}$$

But, $\tau = \dfrac{\lambda}{v}$

To Calculate v (Thermal Velocity)

$$v = \sqrt{\frac{3k_BT}{m}} = \sqrt{\frac{3\times1.38\times10^{-23}\times293}{9.11\times10^{-31}}}$$

$$= \sqrt{1.33\times10^{10}}$$

$$\mathbf{v = 115368.97\ ms^{-1}.}$$

$$\therefore \quad \lambda = \tau v$$

$$= 2.439 \times 10^{-14} \times 115368.97$$

$$\therefore \quad \boldsymbol{\lambda = 2.8138 \times 10^{-9}} \textbf{ m.}$$

Example 5.6

Calculate the drift velocity of electrons in a metal of thickness 1mm across which a potential difference of 1 V is applied. Compare this value with the thermal velocity at temperature 300 K. Given the mobility 0.04 $m^2 V^{-1}s^{-1}$.

Solution:

Given, $t = 1$ mm $= 1\times 10^{-3}$ m ; V = 1 V ; T = 300 K ; $\mu = 0.04\ m^2 V^{-1}s^{-1}$;

$v = ?$; $v_d = ?$

Formula

Thermal Velocity

$$v = \sqrt{\frac{3k_BT}{m}} = \sqrt{\frac{3\times1.38\times10^{-23}\times300}{9.11\times10^{-31}}}$$

$$= \sqrt{1.36333\times10^{10}}$$

$$v = 116762.02\ ms^{-1}$$

or $$\mathbf{v = 116.76 \times 10^3\ ms^{-1}.}$$

Drift Velocity $\mathbf{v_d}$

$$\mu = \frac{v_d}{E}$$

or $$v_d = E\mu$$

But, $E = \frac{V}{t} = \frac{1}{1 \times 10^{-3}} = \mathbf{1000\ Vm^{-1}.}$

$\therefore$ $v_d = 1000 \times 0.04$

$\mathbf{v_d = 40\ ms^{-1}.}$

NOTES

Thus, the thermal velocity is very high compared to the drift velocity.

Example 5.7

Calculate the electrical conductivity of copper. Given atomic weight, density and relaxation time as 63.5, 8.9×10^3 kgm^{-3} and 2.48×10^{-14} s respectively.

Solution:

Given, Atomic Weight = 63.5; Density D = 8.93×10^3 kgm^{-3}; $\tau = 2.48 \times 10^{-14}$ s;

σ = ?

Formula

$$\sigma = \frac{ne^2\tau}{m}$$

To find n

$$n = \text{Number of Free Electrons / Atom} \times \frac{N_A \times D}{\text{Atomic weight}}\ m^{-3}$$

$$= \frac{1 \times 6.023 \times 10^{26} \times 8.93 \times 10^3}{63.5}$$

$$\mathbf{n = 8.4701 \times 10^{28}\ m^{-3}.}$$

$$\therefore \quad \sigma = \frac{8.4701 \times 10^{28} \times \left(1.6 \times 10^{-19}\right)^2 \times 2.48 \times 10^{-14}}{9.11 \times 10^{-31}}$$

$$\sigma = 5.87 \times 10^7\ \Omega^{-1}m^{-1}$$

or $\boldsymbol{\sigma} \mathbf{= 5.87 \times 10^7\ Sm^{-1}.}$ $[\Omega^{-1} = \text{Siemens}]$

Example 5.8

Calculate the drift velocity of electrons in copper and current density in a wire of diameter 0.16×10^{-2} m which carries a current of 10 A. [Given n = 8.48×10^{28} m^{-3}]

Solution:

Given, I = 10 A; Diameter of Wire = 0.16×10^{-2} m

$\therefore$ Radius = 0.8×10^{-2}m; n = 8.48×10^{28} m^{-3}; J = ?; v_d = ?

Formula

The current density is $J = \frac{I}{A}$

$$= \frac{10}{\pi r^2} = \frac{10}{3.14 \times \left(0.8 \times 10^{-2}\right)^2}$$

$$\mathbf{J = 4.9761 \times 10^4\ Am^{-2}.}$$

NOTES

The drift velocity is,

$$v_d = \frac{J}{ne} \qquad [\because J = nev_d]$$

$$= \frac{4.9761 \times 10^4}{8.48 \times 10^{28} \times 1.6 \times 10^{-19}}$$

$$\mathbf{v_d = 3.6675 \times 10^{-6}\ ms^{-1}.}$$

Example 5.9

A uniform silver wire has a resistivity of 1.54×10^{-8} Ωm at room temperature, for an electric field along the wire of 1V/cm. Compute the drift velocity of electron assuming that there are 5.8×10^{28} conduction electrons/m^3. Also calculate the mobility.

Solution:

Given, $\rho = 1.54 \times 10^{-8}$ Ωm; E = 1 V/cm = 100V/m; $n = 5.8 \times 10^{28}\ m^{-3}$; v_d = ?

Formula

$$v_d = \mu E$$

But,

$$\mu = \frac{\sigma}{ne} = \frac{1}{\rho ne} = \frac{1}{1.54 \times 10^{-8} \times 5.8 \times 10^{28} \times 1.6 \times 10^{-19}}$$

$$\mathbf{\mu = 6.99 \times 10^{-3}\ m^2\ V^{-1} s^{-1}}$$

$\therefore$

$$v_d = \mu E$$

$$= 6.99 \times 10^{-3} \times 100$$

or

$$\mathbf{v_d = 0.6997\ ms^{-1}.}$$

Example 5.10

The following datas are given for copper:

(*i*) Density = 8.92×10^3 kg/m^3 (*ii*) Resistivity = 1.73×10^{-8} Ωm

(*iii*) Atomic Weight = 63.5

Calculate the mobility and the average time collision of electrons in copper obeying classical laws.

Solution:

Given, $D = 8.92 \times 10^3$ kg / m^3; Atomic Weight = 63.5; $\rho = 1.73 \times 10^{-8}$ Ωm;

$N_A = 6.02 \times 10^{26}$ per kg mol μ = ?; τ = ?

Formula

$$n = \frac{D \times \text{Avagadro number}}{\text{Atomic weight}} = \frac{8.92 \times 10^3 \times 6.02 \times 10^{26}}{63.5}$$

$$\therefore \quad \mathbf{n = 8.456 \times 10^{28}\ m^{-3}.}$$

NOTES

$$\tau = \frac{m}{ne^2\rho} = \frac{9.1 \times 10^{-31}}{8.456 \times 10^{28} \times (1.6 \times 10^{-19})^2 \times 1.73 \times 10^{-8}}$$

$$\therefore \quad \boldsymbol{\tau = 2.43 \times 10^{-14}\ s.}$$

$$\mu = \frac{1}{\rho ne} = \frac{1}{1.73 \times 10^{-8} \times 8.456 \times 10^{28} \times 1.6 \times 10^{-19}}$$

$$\therefore \quad \boldsymbol{\mu = 0.427 \times 10^{-2}\ m^2V^{-1}s^{-1}.}$$

Example 5.11

Sodium metal with a bcc structure has two atoms/unit cell. The radius of sodium atom is 1.85 Å. Calculate the electrical resistivity at 0°C if the classical value of mean free time at this temperature is 3×10^{-14} sec.

Solution:

Given, $r = 1.85 \times 10^{-10}$m; $\tau = 3 \times 10^{-14}$ sec

Number of atom per unit cell = 2; ρ = ?

Formula

$$\rho = \frac{m}{ne^2\tau}$$

$$n = \frac{\text{Number of atoms per unit cell} \times \text{Number of electrons per unit cell}}{\text{Volume}}$$

$$= \frac{2 \times 1}{a^3} \qquad (\because \text{volume} = a^3)$$

But, $a = \dfrac{4r}{\sqrt{3}}$

$$\therefore \quad a = \frac{4 \times 1.85 \times 10^{-10}}{\sqrt{3}}$$

$$\boldsymbol{a = 4.27 \times 10^{-10}\ m.}$$

$$\therefore \quad n = \frac{2}{(4.27 \times 10^{-10})^3}$$

$$\mathbf{n = 2.57 \times 10^{28}\ m^{-3}.}$$

Electrical resistivity $\rho = \frac{m}{ne^2\tau} = \frac{9.11\times10^{-31}}{2.57\times10^{28}\times\left(1.6\times10^{-19}\right)^2\times3\times10^{-14}}$

NOTES

$\therefore$ $\mathbf{\rho = 4.46 \times 10^{-8}\ \Omega m.}$

Note: The above problem with a different question. Compute electrical resistivity of sodium at 0°C, if the mean free time at this temperature is 3.1×10^{-14} sec. Futher more, sodium builds a bcc lattice with two atoms per unit cell, and the side of the unit cell is 0.429 nm.

Example 5.12

Calculate the free electron concentration, mobility and drift velocity of electrons in an aluminium wire of length 5m and resistance 60 mΩ if it carries a current of 15 A. Assuming that each aluminium atom contributes 3 free electrons for conduction. [Given for aluminium $\rho = 2.7 \times 10^{-8}$ Ωm, atomic weight = 26.98 and density = 2.7×10^3 kg m^{-3}]

Solution:

Given, $\rho = 2.7 \times 10^{-8}$ Ωm; Atomic Weight = 26.98; D = 2.7×10^3 kg m^{-3}

from problem $R = 60 \times 10^{-3}$ W

$l = 5$ m, I = 15 A

Number of Free Electron=3

$n = ?;\ v_d = ?;\ \mu = ?$

Formula n =

$$\frac{\text{Avogadro number} \times \text{Density} \times \text{Number of free electron per atom}}{\text{Atomic weight}}$$

$$= \frac{6.023\times10^{26}\times3\times2.7\times10^3}{26.98}$$

$\therefore$ $\mathbf{n = 1.81 \times 10^{29}}$ **electrons/m^3.**

$$\mu = \frac{1}{ne\rho} = \frac{1}{1.81\times10^{29}\times1.6\times10^{-19}\times2.7\times10^{-8}}$$

$\mathbf{\mu = 1.279 \times 10^{-3}\ m^2\ V^{-1}\ s^{-1}.}$

$$E = \frac{V}{l} = \frac{IR}{l} = \frac{15\times60\times10^{-3}}{5}$$

$\mathbf{E = 0.18\ V/m.}$

$v_d = \mu E = 1.279 \times 10^{-3} \times 0.18$

$\therefore$ $\mathbf{v_d = 2.302 \times 10^{-4}\ m/sec.}$

Example 5.13

Find the resistance of an intrinsic Ge rod of 1cm long 1mm wide and 1mm thick at 300 K. The intrinsic carrier density is 2.5×10^{19} /m^3 at 300 K and the mobility of electron and hole are 0.39 and 0.19 m^{2}V^{-1}s^{-1}.

Solution:

Given, l = 1 cm; b = 1 mm; t = 1 mm; T = 300 K; ρ = ?; R = ?

$n_i = 2.5 \times 10^{19}/m^3$; $\mu_e = 0.39\ m^2V^{-1}s^{-1}$; $\mu_n = 0.19\ m^2V^{-1}s^{-1}$

NOTES

Formula $\sigma = n_i e\ (\mu_e + \mu_h) = 2.5 \times 10^{19} \times 1.6 \times 10^{-19}\ (0.39 + 0.19)$

$\boldsymbol{\sigma = 2.32\ \Omega^{-1}m^{-1}}$**.**

$$\rho = \frac{1}{\sigma} = \frac{1}{2.32}$$

$\boldsymbol{\rho = 0.431\ \Omega m}$**.**

$$R = \frac{\rho l}{A} = \frac{0.431 \times 1 \times 10^{-2}}{1 \times 10^{-3} \times 1 \times 10^{-3}}$$

R = 4310 Ω.

Thermal Conductivity K

The thermal conductivity is defined as the rate of heat flow across a unit area of a conductor per unit temperature gradient.

i.e., $$K = -\frac{Q'}{A\left(\frac{dT}{dx}\right)}$$

Where Q' is the rate of heat flow given by $\left(\frac{dQ}{dt}\right)$

A is the cross sectional area of the conductor.

$\frac{dT}{dx}$ is the temperature gradient.

The –ve sign is optional, which indicates that, the heat flows from higher to lower temperature side.

The unit for thermal conductivity is $\mathbf{W\ m^{-1}K^{-1}}$**.**

In solids, heat transfer takes place by conduction. In the process of heat transfer both electrons and phonons take part. Hence in general, the total thermal conductivity can be written as

$$K_{Total} = K_{Electron} + K_{Phonon}$$

Since, thermal conductivity due to electrons is greater than the thermal conductivity due to phonons in the case of pure metals, the total thermal conductivity is given by $K_{Total} = K_{Electron}$.

Expression for Thermal Conductivity K

Consider a uniform metallic rod AB. Let the surface A be at a higher temperature T, and the surface B be at a lower temperature T-dT as shown in Figure 5.2.

Let the distance of separation between the surface be λ (Mean Free Path). The electrons conduct heat from A to B. During collision, the electrons near A lose their kinetic energy while, the electrons near B gain the energy.

NOTES

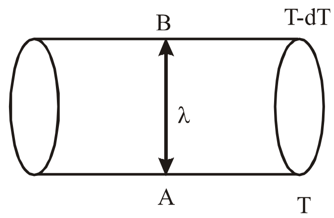


Fig. 5.2 *A Uniform Metallic Rod AB*

Let,

The density of electrons = n

The average thermal velocity = v.

Based on kinetic theory,

The average kinetic energy of an electron at A = $\frac{3}{2}k_BT$ ...[5.25]

Similarly, the average kinetic energy of an electron at B = $\frac{3}{2}k_B(T-dT)$ ...[5.26]

Therefore, the excess kinetic energy carried by electrons from A to B

$$= \frac{3}{2}k_BT - \frac{3}{2}k_B(T - dT)$$

$$= \frac{3}{2}k_BdT \qquad ...[5.27]$$

Since, there is equal probability for the electrons to move in all the six directions (x, y, z) and (–x, –y, –z).

The number of electrons crossing unit area in unit time from A to B = $\frac{1}{6}nv$ ...[5.28]

Therefore, the excess energy transferred from A to B per unit area in unit time

$$= \frac{1}{6}nv \times \frac{3}{2}k_BdT = \frac{1}{4}nv\,k_BdT \qquad ...[5.29]$$

Similarly, the deficiency of energy carried from B to A per unit area in unit time

$$= -\frac{1}{4}nv\,k_BdT \qquad ...[5.30]$$

NOTES

Since, the net energy transferred from A to B per unit area per unit time is the rate of heat flow Q. Then,

$$Q = \frac{1}{4}\ nv\ k_B dT - \left(-\frac{1}{4} nvk_B dT\right)$$

$$= \frac{1}{2}\ nv\ k_B dT. \qquad ...[5.31]$$

But, from the definition of thermal conductivity,

$$K = \frac{Q}{\left(\frac{dT}{dx}\right)}$$

In this case, $dx = \lambda$

$$\therefore \qquad K = \frac{Q}{\frac{dT}{\lambda}} \qquad ...[5.32]$$

Hence, substituting for Q from Equation (5.31) in Equation (5.32), we get

$$K = \frac{\left(\frac{1}{2}\right) nvk_B dT}{\frac{dT}{\lambda}}$$

$$\therefore \qquad \mathbf{K = \frac{nvk_B\lambda}{2}} \qquad ...[5.33]$$

The value of K obtained with the above expression is verified experimentally and the free electron theory is found to be successful in explaining the thermal conductivity.

Note: **Thermal Resistance:** $R_T = \frac{\Delta T}{Q'}$. It is defined as the temperature drop per unit heat flow. It depends on both, the geometry and material. In terms of thermal conductivity, $R_T = \frac{l}{KA}$ where l is the length of the sample and A is the cross sectional area.

Wiedemann-Franz Law

Statement: *This law states that, the ratio of thermal conductivity to the electrical conductivity is directly proportional to the absolute temperature.*

i.e., $$\frac{K}{\sigma} \propto T$$

or $$\frac{K}{\sigma} = LT$$

Where L is a constant called the Lorentz number. Its value is $\boldsymbol{2.44 \times 10^{-8}\ W\Omega K^{-2}}$.

NOTES

Derivation

The electrical conductivity is,

$$\sigma = \frac{ne^2\lambda v}{3k_BT}$$

The thermal conductivity from Equation (5.34) is

$$K = \frac{nvk_B\lambda}{2}$$

$$\therefore \quad \frac{K}{\sigma} = \frac{nvk_B\lambda}{2\left(\frac{ne^2\lambda v}{3k_BT}\right)} = \frac{nvk_B\lambda.3k_BT}{2ne^2\lambda v} = \frac{3}{2}\,\frac{k_B^2}{e^2}\,T$$

$$\therefore \quad \frac{K}{\sigma} = \frac{3}{2}\left(\frac{k_B}{e}\right)^2 T = L\,T, \text{ where } L = \frac{3}{2}\left(\frac{k_B}{e}\right)^2.$$

Thus, Wiedemann-Franz law is obtained.

$\boldsymbol{L = \frac{3}{2}\left(\frac{k_B}{e}\right)^2 = 1.12 \times 10^{-8}\ W\Omega K^{-2}}$ *is known as the Lorentz number.*

The above value of Lorentz number based on classical concept does not agree with the experimental value. Hence, the assumption that all the free electrons of a metal participate in thermal conductivity is not correct.

The actual experimental value of the Lorentz number is ***2.44×10^{-8} $W\Omega K^{-2}$.***

Thus, there is a discrepancy in the value of L between classical theory and the experimental value. This discrepancy gets eliminated on applying quantum theory.

Success of Free Electron Theory

1. It verifies ohm's law.
2. It explains the thermal and electrical conductivities of metals.
3. It is used to deduce Wiedemann-Franz law.
4. It explains the optical properties of metals.

5.3 FREE ELECTRON GAS ON THREE DIMENSIONS

1. The theoretical value obtained for specific heat and electronic specific heat of metals based on this theory is not in agrement with the experimental value.
2. The classical free electron theory is not able to explain the electrical conductivity of semiconductors and insulators.

3. According to classical theory, $\frac{K}{\sigma T}$ is constant at all temperatures. But, this is not constant at low temperature.
4. The theoretical value of paramagnetic susceptibility (χ) is greater than the experimental value also, ferromagnetism cannot be explained.
5. The phenomena such as photoelectric effect, compton effect and black body radiation could not be explained by this theory.

NOTES

Example 5.14

Find the thermal conductivity of copper at 20°C with a free electron density of 8.48×10^{28} m^{-3}. The thermal velocity of copper at 20°C is 1.1536×10^5 ms^{-1}. With a mean free path of 2.8138 nm.

Solution:

Given, $n = 8.48 \times 10^{28}$ m^{-3}; $\lambda = 2.8138$ nm $= 2.8138 \times 10^{-9}$m;

$v = 1.1536 \times 10^5$ ms^{-1}; K = ?

Formula

$$K = \frac{1}{2} nvk_B\lambda$$

$$= \frac{1}{2} \times 8.48 \times 10^{28} \times 1.1536 \times 10^5 \times 1.38 \times 10^{-23} \times 2.8138 \times 10^{-9}$$

$$= \frac{1}{2} \times 379.85$$

$$\mathbf{K = 189.92\ Wm^{-1}K^{-1}.}$$

Example 5.15

A brass disk of electrical resistivity 50×10^{-8} Ωm conducts heat from a heat source to a heat sink at a rate of 10W. If its diameter is 26 mm with thickness 35 mm. Compute the thermal conductivity and thermal resistance at 300 K.

Solution:

Given, $\rho = 50 \times 10^{-8}$ Ωm; T = 300 K

Diameter = 26 mm = 26×10^{-3} m

∴ Radius = 13×10^{-3} m

Thickness = 35 mm = 35×10^{-3} m

Formula

The thermal resistance is given by

$$R_T = \frac{l}{KA}$$

But, $$K = \sigma LT = \frac{LT}{\rho} = \frac{2.44 \times 10^{-8} \times 300}{50 \times 10^{-8}}$$

∴ $$\mathbf{K = 14.64\ Wm^{-1}K^{-1}.}$$

Therefore, the thermal resistance is,

$$R_T = \frac{l}{KA}$$

NOTES

$\left[\because A = \pi r^2\right]$

$$= \frac{35\times10^{-3}}{14.64\times3.14\times\left(13\times10^{-3}\right)^2} = \frac{35\times10^{-3}}{7.768\times10^{-3}}$$

$$\mathbf{R_T = 4.505\ KW^{-1}.}$$

Example 5.16

The thermal and electrical conductivity of copper at 20°C are 380 $Wm^{-1}K^{-1}$ and $5.87 \times 10^7\ \Omega^{-1}m^{-1}$ respectively. Calculate the Lorentz number.

Solution:

Given, $\sigma = 5.87 \times 10^7\ \Omega^{-1}m^{-1}$; $K = 380\ Wm^{-1}K^{-1}$; T = 20°C = 293K; L = ?

Formula

$$\frac{K}{\sigma} = LT$$

$$\therefore \quad L = \frac{K}{\sigma T} = \frac{380}{5.87\times10^7\times293}$$

$$\therefore \quad \mathbf{L = 2.2094 \times 10^{-8}\ W\Omega K^{-2}}$$

Example 5.17

Copper has electrical conductivity at 300K as 6.40×10^7 mho m^{-1}. Calculate the thermal conductivity of copper.

Solution:

Given, $\sigma = 6.40 \times 10^7$ mho m^{-1}; T = 300K; K = ?

Formula

$$\frac{K}{\sigma} = LT$$

$$\therefore \quad K = \sigma LT$$

$$= 6.4 \times 10^7 \times 2.44 \times 10^{-8} \times 300$$

$$\mathbf{K = 468.48\ Wm^{-1}k^{-1}.}$$

5.4 FERMI ENERGY

We know in an intrinsic semiconductor

$$n_e = n_h$$

i.e.,

{Density of electrons in the conduction band} = {Density of holes in the valence band}

Therefore,

$$2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2} e^{\left(\frac{E_F - E_c}{k_B T}\right)} = 2\left(\frac{2\pi m_h^* k_B T}{h^2}\right)^{3/2} e^{\left(\frac{E_v - E_F}{k_B T}\right)}$$

or

$$(m_e^*)^{3/2} e^{\left(\frac{E_F - E_c}{k_B T}\right)} = (m_h^*)^{3/2} e^{\frac{E_v - E_F}{k_B T}}$$

NOTES

Rearranging the above equation we get,

$$e^{\left(\frac{2E_F}{k_B T}\right)} = \left(\frac{m_h^*}{m_e^*}\right)^{3/2} e^{\left(\frac{E_v + E_c}{k_B T}\right)} \qquad \text{...(5.34)}$$

Taking logarithm on both sides,

$$\frac{2E_F}{k_B T} = \frac{3}{2} \ln\left(\frac{m_h^*}{m_e^*}\right) + \frac{E_v + E_c}{k_B T}$$

[The RHS of Equation (5.33) has been written using the formula ln (ab) = ln$a$ + lnb].

Note: In is natural base of logarithm $\ln N = \log_e^N = 2.302 \log_{10}^N$.

$$\therefore \quad ME_F = \frac{3k_B T}{4} \ln\left(\frac{m_h^*}{m_e^*}\right) + \frac{E_v + E_c}{2} \qquad \text{...(5.34)}$$

when $m_e^* = m_h^*$, the above Equation gets reduced to

$$E_F = \frac{E_v + E_c}{2}, \text{ Since } \quad \ln(1) = 0 \qquad \text{...(5.35)}$$

Thus, the Fermi level is in the middle of the band gap, i.e., $E_F = \frac{E_g}{2}$. ...(5.36)

As shown in Figure 5.3(a) E_g lies half way between the top of valence band and bottom of conduction band.

Dependence of E_F on Temperature

The variation of Fermi level with temperature for an intrinsic semiconductor is shown in Figure 5.3. At T = 0 K, the Fermi level lies exactly in the middle of forbidden gap as shown in Figure 5.3(a).

At low temperature region, E_F is practically independent of temperature. But, there is a slight variation in E_F in the high temperature region. The reason is, in actual case $m_e^* > m_h^*$. Thus, the term $\ln\left(\frac{m_h^*}{m_e^*}\right)$ begins to contribute slightly. This results in a small increase in the magnitude of E_F. Thus the Fermi level gets raised slightly as shown in Figure 5.3(b) as T increases.

NOTES

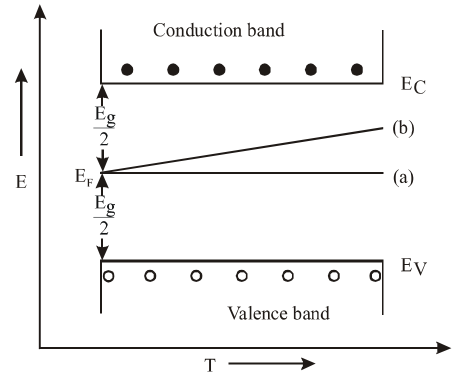


Fig. 5.3 *Position of Fermi Level in an Intrinsic Semiconductor at Various Temperatures*

5.5 HALL EFFECT

If a specimen (metal or semiconductor) carrying a current I is placed in a transverse magnetic field B, an electric field E is induced in the direction perpendicular to both I and B. This phenomenon is known as Hall effect and the generated voltage is called the Hall voltage.

Theory

Consider a rectangular slab of a n-type semiconductor material which carries a current I along the positive X-direction as shown in Figure 5.4. In an n-type semiconductor electrons are the majority carries.

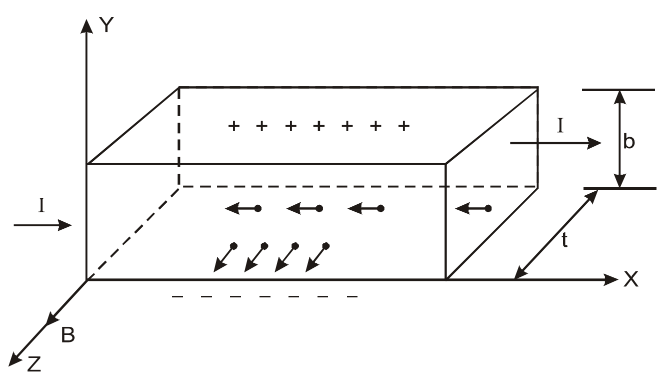


Fig. 5.4 *Hall Effect*

Let a magnetic field B is applied along the positive Z-direction. Under the influence of this magnetic field, the electrons experience a force called Lorentz force given by

$$F_L = -Bev_d \qquad ...(5.37)$$

where e is the magnitude of charge of the electrons and v_d is the drift velocity.

This Lorentz force is exerted on the electrons in the negative Y-direction.

The direction of this force is given by Fleming's left hand rule. Thus, the electrons are therefore deflected downwards and collect at the bottom surface of the specimen.

On the other hand, the top edge of the specimen becomes positively charged due to the loss of electrons. Hence, a potential called the Hall voltage V_H is developed between the upper and lower surfaces of the specimen which establishes an electric field E_H called the Hall field across the specimen in the negative Y-direction.

This electric field excerts an upward force on the electron and is given by

$$F_E = -eE_H \qquad ...(5.38)$$

At equilibrium, the Lorentz force and the electric force gets balanced. Hence,

$$F_E = F_L$$

Therefore, from Equations (5.38) and (5.39)

$$-eE_H = -Bev_d$$

or $$E_H = Bv_d \qquad ...(5.39)$$

If b is the width (i.e., the distance between the top and bottom surface) of the specimen, then

$$E_H = \frac{V_H}{b} \qquad ...(5.40)$$

or $$V_H = E_H\, b \qquad ...(5.41)$$

and $$V_H = Bv_d b \qquad ...(5.42)$$

Let t be the thickness of the specimen along the Z direction. Therefore, its area of cross-section normal to the direction of current is bt.

If J is the current density, then,

$$J = \frac{I}{bt} \qquad ...(5.43)$$

But, J can also be expressed as

$$J = -n_e\, ev_d$$ where n_e is the density of electrons.

...(5.44)

$$\therefore \quad v_d = \frac{-J}{n_e e} \qquad ...(5.45)$$

Hence, substituting Equation (5.44) in Equation (5.45)

$$V_H = -Bb\,\frac{J}{n_e e} \qquad ...(5.46)$$

But, V_H is also equal to E_H b

$$\therefore \quad E_H\, b = -Bb\frac{J}{n_e e}$$

or $$E_H = \frac{-BJ}{n_e e} \qquad ...(5.47)$$

NOTES

Note: The polarity of Hall voltage for an n-type semiconductor is positive at the top surface. For a p-type semiconductor the polarity of Hall voltage is positive at the bottom surface. The polarity of the Hall voltage developed at the top and bottom surface of the specimen can be identified by using probes.

Hall Coefficient R_H

The Hall effect is described by means of Hall coefficient R_H. It is given by

$$R_H = \frac{1}{ne}$$

where n is in general, the carrier concentration.

R_H for n-Type and p-Type Material

A negative sign is used while denoting the Hall coefficient for an n-type material i.e.,

It is given by $$R_H = -\frac{1}{n_e e} \quad ...(5.48)$$

where n_e is the density of electrons.

But, for a p-type material a positive sign is used to denote the Hall coefficient. i.e.,

It is given by $$R_H = \frac{1}{n_h e} \quad ...(5.49)$$

where n_h is the density of holes.

Therefore, Equation (5.49) can be written as

$$E_H = BJ\, R_H$$

i.e., $$R_H = \frac{E_H}{JB} \quad ...(5.50)$$

But, we know $E_H = \frac{V_H}{b}$ and $J = \frac{I}{bt}$. Hence Equation (5.50) becomes,

$$R_H = \frac{V_H bt}{IBb}$$

$$\therefore \quad R_H = \frac{V_H t}{IB} \quad ...(5.51)$$

Since, the quantities V_H, t, I and B are measurable, the Hall coefficient R_H can be determined.

Experimental Determination of Hall Coefficient

A rectangular slab of thickness t and width b is placed at right angles to a magnetic field B. A known current I is passed through the material along the X-axis by connecting it to a dc battery, key, a rheostat and a milliammeter as shown in Figure 5.5.

A calibrated voltmeter connected between the opposite ends of the slab measures the Hall voltage V_H. Thus, the Hall field is given by

$$E_H = \frac{V_H}{b}$$

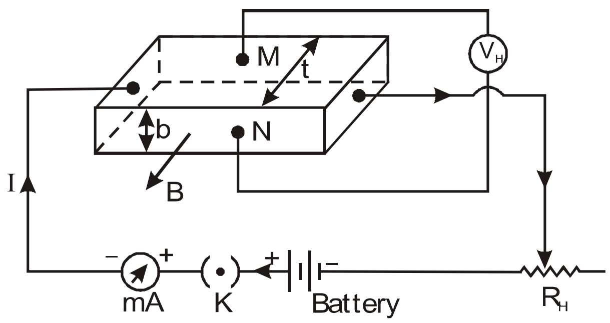


Fig. 5.5 *Experimental Setup to Determine Hall Coefficient*

The current density is given by

$$J = \frac{I}{bt}$$

Thus, R_H can be calculated using the formula

$$R_H = \frac{V_H t}{IB}$$

Mobility Determination

For an n-type material the conductivity is given by

$\sigma_e = n_e e\,\mu_e$ where μ_e is the mobility of electrons.

$$\therefore \quad \mu_e = \frac{\sigma_e}{n_e e} \quad ...(5.52)$$

$$\text{or} \quad \mu_e = -\sigma_e R_H \quad ...(5.53)$$

Similarly, for a p -type material, the conductivity is given by

$\sigma_h = n_h e\,\mu_h$ where μ_h is the mobility of holes.

$$\therefore \quad \mu_h = \frac{\sigma_h}{n_h e} \quad ...(5.54)$$

$$\text{or} \quad \mu_h = \sigma_h R_H \quad ...(5.55)$$

In the above discussion, it is assumed that all the charge carriers travel with average velocity. But actually, the charge carriers have a random thermal distribution in velocity.

With this distribution taken into consideration, R_H is defined in general as

$$R_H = \frac{3\pi}{8ne} = \frac{1.18}{ne} \quad ...(5.56)$$

Therefore, Equations (5.54) and (5.56) can be written as

$$\mu_e = \frac{-\sigma_e R_H}{1.18} \quad \text{(For n-type material)} \qquad ...(5.57)$$

And $$\mu_h = \frac{\sigma_h R_H}{1.18} \quad \text{(For p-type material)} \qquad ...(5.58)$$

NOTES

Applications of Hall Effect

The Hall effect can be used for:

1. Determining whether a semiconductor is n-type or p-type.
2. Determining the carrier concentration and mobility.
3. Determining the magnetic field B in terms of Hall voltage V_H.
4. Designing the gauss meter and electronic meters based on Hall voltage.

Example 5.18

The conductivity and the Hall coefficient of a n-type silicon specimen are 112 $\Omega^{-1}m^{-1}$ and 1.25×10^{-13} m^3C^{-1} respectively. Calculate the charge carrier density and electron mobility.

Solution:

Given, $\sigma_e = 112\ \Omega^{-1}m^{-1}$; $R_H = 1.25 \times 10^{-13}\ m^3C^{-1}$; n_e = ? and μ_e = ?

Formula $$\mu_e = \sigma_e\ R_H$$

$$= 112 \times 1.25 \times 10^{-4} = \mathbf{0.014\ m^2V^{-1}s^{-1}}.$$

We know $$\mu_e = \frac{\sigma_e}{n_e e}.$$

$\therefore$ $$n_e = \frac{\sigma_e}{\mu_e e} = \frac{112}{0.014 \times 1.6 \times 10^{-19}}$$

$$= \frac{112}{2.24 \times 10^{-21}} = \mathbf{5 \times 10^{22}\ electrons/m^3}.$$

Example 5.19

A semiconducting crystal 12mm long, 1mm wide and 1mm thick has a magnetic flux density of 0.5Wb/m^2 applied from front to back, perpendicular to largest faces. When a current of 20mA flows lengthwise through the specimen, the voltage measured across its width is found to be 37 μv. What is the Hall coefficient of semiconductor and the density of charge carrier.

Solution:

Given,

l = 12 mm = 12×10^{-3} m; t = 1 mm = 1×10^{-3} m

b = 1 mm = 1×10^{-3} m, I = 20 m A = 20×10^{-3} A

v_H = 37 μV = 37×10^{-6} V, B = 0.5 Wb/m^2.

R_H = ? and n = ?

We know

$$R_H = \frac{V_H t}{IB}$$

$$= \frac{37\times10^{-6}\times1\times10^{-3}}{20\times10^{-3}\times0.5} = \frac{3.7\times10^{-8}}{0.01}$$

$$\mathbf{R_H = 3.7 \times 10^{-6}\ C^{-1}\ m^3.}$$

NOTES

Example 5.20

A silicon plate of thickness 1mm, breadth 10mm and length 100mm is placed in a magnetic field of 0.5 Wb/m² acting perpendicular to its thickness. If 10^{-2} A current flows along its length, calculate the Hall coefficient, if Hall voltage developed is 1.83 mV.

Solution:

Given,

$t = 1\text{ mm} = 1 \times 10^{-3}\text{ m}$, $b = 10\text{ mm} = 10 \times 10^{-3}\text{ m}$

$l = 100\text{ mm} = 100 \times 10^{-3}\text{ m}$, $B = 0.5\text{ Wb/m}^2$

$I = 10^{-2}\text{ A}$; $V_H = 1.83\text{ mV} = 1.83 \times 10^{-3}\text{ V}$.

$R_H = ?$

Formula

$$R_H = \frac{V_H t}{IB} = \frac{1.83\times10^{-3}\times1\times10^{-3}}{10^{-2}\times0.5}$$

$$\therefore \quad \mathbf{R_H = 3.66 \times 10^{-4}\ m^3C^{-1}.}$$

Example 5.21

The Hall coefficient of certain silicon specimen was found to be -7.35×10^{-5} m²C⁻¹ from 100 to 400 K. Determine the nature of the semiconductor if the conductivity was found to be 200 $\Omega^{-1}m^{-1}$. Calculate the density and mobility of the charge carrier.

Solution:

Given, $R_H = -7.35 \times 10^{-5} m^3C^{-1}$; $\sigma = 200\ \Omega^{-1}m^{-1}$; $n_e = ?$ and $\mu_e = ?$

The negative sign of the Hall coefficient indicates that the nature of the semiconductor is n-type.

Formula $$n_e = \frac{1}{R_H e} = \frac{1}{7.35\times10^{-5}\times1.6\times10^{-19}}$$

$$\therefore \quad \mathbf{n_e = 8.503 \times 10^{22}\ electrons / m^3.}$$

Mobility $$\mu_e = \frac{\sigma}{n_e e} = \frac{200}{8.503\times10^{22}\times1.6\times10^{-19}}$$

$$\therefore \quad \mathbf{\mu_e = 14.7006 \times 10^{-3} m^2V^{-1}s^{-1}.}$$

or

$$\mu_e = \sigma R_H$$

$$= 200 \times 7.35 \times 10^{-5}$$

$$\therefore \quad \mathbf{\mu_e = 14.7 \times 10^{-3} m^2V^{-1}s^{-1}.}$$

Example 5.22

A n-type semiconductor has Hall coefficient = 4.16 × 10^{-4} m^3C^{-1}. The conductivity is 108 $\Omega^{-1}m^{-1}$. Calculate its charge carrier density n_e and electron mobility at room temperature.

Solution:

Given, $R_H = 4.16 \times 10^{-4}\ m^3C^{-1}$; $\sigma = 180\Omega^{-1}m^{-1}$; n_e = ? and μ_ε = ?

$$R_H = \frac{1.18}{n_e e} \qquad \text{(with correction factor for } R_H)$$

$$\therefore \quad n_e = \frac{1.18}{R_H e} = \frac{1.18}{4.16\times10^{-4}\times1.6\times10^{-19}}$$

$$\therefore \quad \mathbf{n_e = 1.772 \times 10^{22}/m^3.}$$

We know $\sigma = n_e e \mu_e$

$$\therefore \quad \mu_e = \frac{\sigma}{n_e e} = \frac{180}{1.772\times10^{22}\times1.6\times10^{-19}}$$

$$\therefore \quad \mathbf{M\mu_e = 0.06348\ m^2V^{-1}s^{-1}.}$$

Example 5.23

A rectangular plane sheet of doped silicon has dimensions of 1cm along Y – direction, and 0.5mm along Z – direction. Hall probes are attached on its two surfaces parallel to X – Z Plane and a magnetic field of flux density 0.7 Wb/m^2 is applied along Z – direction. A current of 1mA is flowing in it in the X – direction. Calculate the Hall voltage measured by the probes if the Hall coefficient of the material is 1.25 × 10^{-3} m^3 C^{-1}.

Solution:

Given, B = 0.7 Wb/m^2; I = 1 × 10^{-3} A; R_H = 1.25 × 10^{-3} m^3C^{-1}; b = 1cm = 1 × 10^{-2}m

t = 0.5 mm = 0.5 × 10^{-3} m; V_H = ?

$$V_H = \frac{R_H IB}{t} = \frac{1.25\times10^{-3}\times1\times10^{-3}\times0.7}{0.5\times10^{-3}}$$

$$= 1.75 \times 10^{-3}\ V$$

or $\mathbf{V_H = 1.75\ mV.}$

Example 5.24

The Hall coefficient of a specimen of a doped silicon is found to be 3.66×10^{-4} m^3C^{-1}. The resistivity of the specimen is 8.93 ×$10^{-3}\Omega$m. Find the mobility and density of the charge carrier.

Solution:

Given, $R_H = 3.66 \times 10^{-4}\ m^3C^{-1}$; $\rho = 8.93 \times 10^{-3}\Omega m$; μ = ? and n = ?

Formula

$$R_H = \frac{1}{ne}$$

$$\therefore \qquad n = \frac{1}{R_H e} = \frac{1}{3.66 \times 10^{-4} \times 1.6 \times 10^{-19}}$$

$$\mathbf{n = 1.7076 \times 10^{22} / m^3.}$$

NOTES

Mobility $\qquad \mu = \sigma R_H$

$$\text{or} \qquad \mu = \frac{R_H}{\rho}$$

$$\therefore \qquad \mu = \frac{3.66 \times 10^{-4}}{8.93 \times 10^{-3}}$$

$$\text{or} \qquad \boldsymbol{\mu = 0.0409\ m^2V^{-1}s^{-1}.}$$

Example 5.25

An electric field of 100 V/m is applied to a sample of n-type semiconductor whose Hall coefficient is $-0.0125\ m^3C^{-1}$. Determine the current density in the sample, assuming electron mobility to be $0.36\ m^2V^{-1}s^{-1}$.

Solution:

Given, $R_H = -0.0125\ m^3C^{-1}$; $\mu_e = 0.36\ m^2V^{-1}s^{-1}$; $E_H = 100$ V/m; J = ?

We know

$$R_H = \frac{1}{n_e e}$$

$$\therefore \qquad n_e = \frac{1}{R_H e} = \frac{1}{0.0125 \times 1.6 \times 10^{-19}}$$

$$\mathbf{n_e = 5 \times 10^{20} / m^3.}$$

$$\sigma_e = n_e e\, \mu_e = 5 \times 10^{20} \times 1.6 \times 10^{-19} \times 0.36$$

$$\therefore \qquad \boldsymbol{\sigma_e = 28.8\ \Omega^{-1}\ m^{-1}.}$$

We also know $\qquad J = \sigma_e E$

$$\therefore \qquad J = 28.8 \times 100$$

$$\text{or} \qquad \mathbf{J = 2880\ A/m^2.}$$

Check Your Progress

1. Explain the electrical properties of metals.
2. Define the Ohm's law.
3. Elaborate on the current density.
4. Interpret the classical free electron theory of metals.
5. Differentiate between the relaxation time and mean collision time.
6. State the Wiedemann-Franz law.
7. Define the free electron gas on three dimensions.
8. Elaborate on the Hall effect.

5.6 ANSWERS TO CHECK YOUR PROGRESS QUESTIONS

NOTES

1. Metals have high electrical and thermal conductivities. Above Debye's temperature, the ratio of thermal and electrical conductivities is directly proportional to the absolute temperature, and is known as Wiedemann-Franz law.
2. When an electric current flows through a material, the magnitude of the current flowing through the material is given by Ohm's law:
$$I = \frac{V}{R}.$$
3. Current density is defined as the current per unit area of cross-section of an imaginary plane held normal to the direction of flow of current in a current carrying conductor.
4. This theory was developed by Drude and Lorentz. Even though it is a macroscopic theory it successfully explained most of the properties of metals. In this theory, the free electrons in a metal are treated like molecules in a gas and Maxwell-Boltzmann statistics is applied.
5. Relaxation time (τ) is defined as the time taken by the free electron to reach its equilibrium position from its disturbed position just when the field is switched off while mean collision time (τ_c) is the average time between two consecutive collisions of an electron with the lattice points is called collision time.
6. This law states that, the ratio of thermal conductivity to the electrical conductivity is directly proportional to the absolute temperature, i.e.,
$$\frac{K}{\sigma} \propto T$$
$$\frac{K}{\sigma} = LT.$$
7. The theoretical value obtained for specific heat and electronic specific heat of metals based on this theory is not in agreement with the experimental value. The classical free electron theory is not able to explain the electrical conductivity of semiconductors and insulators.
8. If a specimen (metal or semiconductor) carrying a current I is placed in a transverse magnetic field B, an electric field E is induced in the direction perpendicular to both I and B. This phenomenon is known as Hall effect and the generated voltage is called the Hall voltage.

5.7 SUMMARY

- Metals have high electrical and thermal conductivities. Above Debye's temperature, the ratio of thermal and electrical conductivities is directly

proportional to the absolute temperature, and is known as Wiedemann-Franz law.

- When an electric current flows through a material, the magnitude of the current flowing through the material is given by Ohm's law:

$$I = \frac{V}{R}$$.

- Current density is defined as the current per unit area of cross-section of an imaginary plane held normal to the direction of flow of current in a current carrying conductor.
- Classical free electron theory of metals was developed by Drude and Lorentz. Even though it is a macroscopic theory it successfully explained most of the properties of metals. In this theory, the free electrons in a metal are treated like molecules in a gas and Maxwell-Boltzmann statistics is applied.
- Relaxation time is defined as the time taken by the free electron to reach its equilibrium position from its disturbed position just when the field is switched off.
- Mean collision time is the average time between two consecutive collisions of an electron with the lattice points is called collision time.
- The theoretical value obtained for specific heat and electronic specific heat of metals based on this theory is not in agreement with the experimental value.
- The classical free electron theory is not able to explain the electrical conductivity of semiconductors and insulators.
- If a specimen (metal or semiconductor) carrying a current *I* is placed in a transverse magnetic field *B*, an electric field *E* is induced in the direction perpendicular to both *I* and *B*. This phenomenon is known as Hall effect and the generated voltage is called the Hall voltage.

5.8 KEY WORDS

- **Electrical properties of metals:** Metals have high electrical and thermal conductivities. Above Debye's temperature, the ratio of thermal and electrical conductivities is directly proportional to the absolute temperature, and is known as Wiedemann-Franz law.
- **Relaxation time:** It is defined as the time taken by the free electron to reach its equilibrium position from its disturbed position just when the field is switched off.
- **Mean collision time:** It is the average time between two consecutive collisions of an electron with the lattice points is called collision time.
- **Mean free path :** It is the average distance travelled by the conduction electron between successive collisions with the lattice ions.

NOTES

- **Thermal conductivity *K*:** The thermal conductivity is defined as the rate of heat flow across a unit area of a conductor per unit temperature gradient.
- **Hall effect:** If a specimen (metal or semiconductor) carrying a current I is placed in a transverse magnetic field B, an electric field E is induced in the direction perpendicular to both I and B.

5.9 SELF ASSESSMENT QUESTIONS AND EXERCISES

Short-Answer Questions

1. Define the electrical properties of metals.
2. Explain the Ohm's law.
3. Elucidate on the current density.
4. State the classical free electron theory of metals.
5. Differentiate between the relaxation time and mean collision time.
6. Elaborate on the Wiedemann-Franz law.
7. Describe the free electron gas on three dimensions.
8. Define the Hall effect.

Long-Answer Questions

1. Describe the electrical properties of metals.
2. Briefly define the classical free electron theory of metals giving suitable examples.
3. Differentiate between the relaxation time and mean collision time.
4. Analyse the Wiedemann-Franz law.
5. Explain the free electron gas on three dimensions giving suitable examples.
6. Discuss briefly the Hall effect.

5.10 FURTHER READINGS

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UNIT 6 BAND THEORY OF SOLIDS

NOTES

Structure

6.0 Introduction
6.1 Objectives
6.2 Band Theory of Solids
6.3 Kronig-Penny Model
6.4 Semiconductor
6.5 Classifications of Semiconductors
    6.5.1 Intrinsic Semiconductors
    6.5.2 Extrinsic Semiconductors
6.6 Fermi Energies of Impurity Semiconductors
6.7 Answers to Check Your Progress Questions
6.8 Summary
6.9 Key Words
6.10 Self Assessment Questions and Exercises
6.11 Further Readings

6.0 INTRODUCTION

A solid has an infinite number of allowed bands, just as an atom has infinitely many energy levels. However, most of the bands simply have too high energy, and are usually disregarded under ordinary circumstances. Conversely, there are very low energy bands associated with the core orbitals. These low-energy core bands are also usually disregarded since they remain filled with electrons at all times, and are therefore inert. Likewise, materials have several band gaps throughout their band structure.

In condensed matter physics, the electronic band structure of a solid describes the range of energy levels that electrons may have within it, as well as the ranges of energy that they may not have (called band gaps or forbidden bands). Band theory has been successfully used to explain many physical properties of solids, such as electrical resistivity and optical absorption, and forms the foundation of the understanding of all solid-state devices (transistors, solar cells, etc.).

Band theory derives these bands and band gaps by examining the allowed quantum mechanical wave functions for an electron in a large, periodic lattice of atoms or molecules. The formation of bands is mostly a feature of the outermost electrons (valence electrons) in the atom, which are the ones involved in chemical bonding and electrical conductivity. The inner electron orbitals do not overlap to a significant degree, so their bands are very narrow.

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Although, electronic band structures are usually associated with crystalline materials, quasi-crystalline and amorphous solids may also exhibit band gaps. These are somewhat more difficult to study theoretically since they lack the simple symmetry of a crystal, and it is not usually possible to determine a precise dispersion relation. As a result, virtually all of the existing theoretical work on the electronic band structure of solids has focused on crystalline materials.

In this unit, you will study about the band theory of solids, Kronig–Penney model, semiconductors, classification of semiconductors, and Fermi energies of impurity semiconductors.

6.1 OBJECTIVES

After going through this unit, you will be able to:

- Understand the band theory of solids
- Explain the Kronig–Penney model
- Comprehend the semiconductors and their classifications
- Analyse the Fermi energies of impurity semiconductors

6.2 BAND THEORY OF SOLIDS

In the case of a single isolated atom, the electron in any orbit as shown in Figure 6.1 have a definite energy. As a result, they occupy discrete energy levels, as shown in Figure 6.2(a).

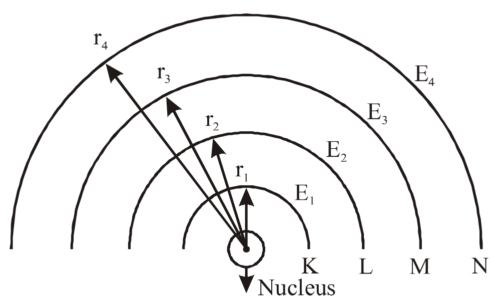


Fig. 6.1 *The energy Levels of a Single Isolated Atom*

The pauli exclusion principle allows each energy level to contain only two electrons. For example, the 2s level of a single atom contains one energy level with two electrons and 2p level contains 3 energy levels with two electrons in each level thus, with a total of six electrons as shown in Figure 6.2(a).

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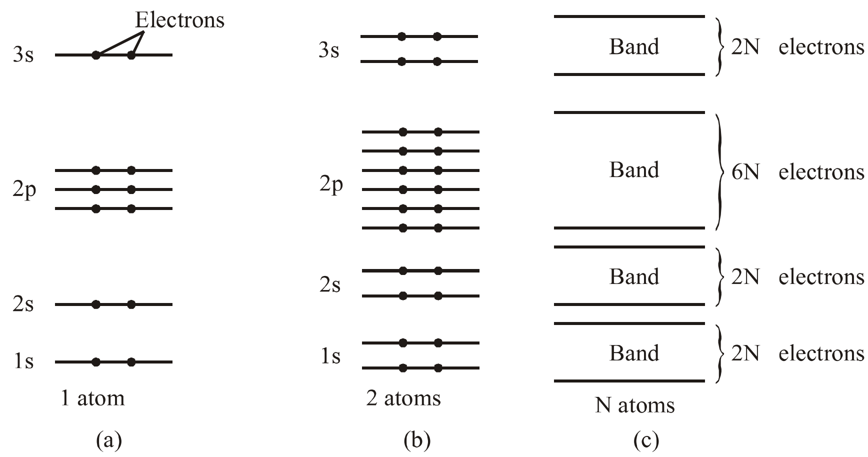


Fig. 6.2 *The Energy Levels Broaden Into Energy Bands*

Band Structure in Solid

Let us consider the formation of bands in a solid sodium.

The single energy level of an isolated sodium (Z = 11) based on the electron configuration $1s^2\ 2s^2\ 2p^6\ 3s^1$ is shown in Figure 6.2(a).

When an another sodium is brought close to it, the electrons will be subjected to the effect of an additional field. As a result, each energy level is split in to two as shown in Figure 6.2(b). Similarly, when three atoms come close together, the original level splits into three levels and so on.

More generally, when a solid is formed by bringing N atoms together, the Pauli principle still demands that only two electrons in the entire solid should have the same energy. Hence, in a solid the different split energy levels of electrons come together to form continuous bands of energies as shown in Figure 6.2(c).

Consequently, the 2s band in a solid sodium contain N discrete energy levels and 2N electrons, two in each energy level. Similarly, each of the 2p level contain N energy levels and 2N electrons. Hence, a broad 2p band will contain 3N energy levels and 6N electrons since the three 2p bands overlap.

Hence in general, each energy band has a total of N individual levels and each energy band can hold a maximum of $2(2l + 1)$ N electrons.

[Each energy level can hold $2\ (2l + 1)$ electrons. 2 corresponds to the electrospin and $(2l + 1)$ corresponds to the orientation of the electron orbital angular momentum].

The result is that, electrons in any orbit of atom within a solid can have a range of energies rather than a single value. *Thus, the range of energies possessed by an electron in a solid is known as energy band.* i.e., Each energy level of an isolated atom becomes a band in a solid as shown in Figure 6.2(c).

6.3 KRONIG-PENNY MODEL

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The Kronig–Penney model (named after Ralph Kronig and William Penney) is a simple, idealized quantum-mechanical system that consists of an infinite periodic array of rectangular potential barriers.

Consider a particle of mass m having a total energy E moving in a one-dimensional potential $V(x)$. The state of the particle described by the wavefunction $\psi(x)$ satisfies the time-independent Schrödinger equation,

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\,\psi(x) = 0 \qquad \ldots(6.1)$$

The solutions of the above equation give the energy eigenfunctions $\psi_n(x)$ belonging to different energy eigenvalues E_n for the particle.

Equation (6.1) can be solved exactly only when (i) the potential function $V(x)$ is stated explicitly and (ii) the boundary conditions imposed on the system, i.e., on the wavefunction $\psi(x)$ are known exactly.

The nature of the states of the particle is determined completely by the energy of the particle and the nature of the potential function $V(x)$. We encounter the following results with respect to the energy eigenvalues and states:

(i) The eigenvalues form a *discrete-spectrum* corresponding to *bound* states.

(ii) The eigenvalues form a *continuous spectrum* corresponding to unbound states.

(iii) The eigenvalues form a mixed spectrum consisting of a discrete spectrum for some range of energy E and a continuous spectrum outside that range.

In the sections to follow we shall illustrate the above results by considering some important problems of one-dimensional motion.

The important properties of one-dimensional motion that we find are:

(i) In case of bound states, the energy spectrum is not only discrete but is non-degenerate also.

(ii) The eignfunction $\psi_n(x)$ for a bound state has 'n' number of nodes if the ground state corresponds to $n = 0$ and $(n - 1)$ number of nodes if the ground state corresponds to $n = 1$.

6.4 SEMICONDUCTOR

Semiconductors are defined by their unique electric conductive behaviour, somewhere between that of a conductor and an insulator. A semiconductor material

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has an electrical conductivity value falling between that of a conductor, such as metallic copper, and an insulator, such as glass. Its resistivity falls as its temperature rises; metals behave in the opposite way. Its conducting properties may be altered in useful ways by introducing impurities ("Doping") into the crystal structure. When two differently-doped regions exist in the same crystal, a semiconductor junction is created.

The behaviour of charge carriers, which include electrons, ions and electron holes, at these junctions is the basis of diodes, transistors and most modern electronics. Some examples of semiconductors are silicon, germanium, gallium arsenide, and elements near the so-called "Metalloid Staircase" on the periodic table. After silicon, gallium arsenide is the second most common semiconductor and is used in laser diodes, solar cells, microwave-frequency integrated circuits, and others. Silicon is a critical element for fabricating most electronic circuits.

Semiconductor devices can display a range of useful properties, such as passing current more easily in one direction than the other, showing variable resistance, and sensitivity to light or heat. Because the electrical properties of a semiconductor material can be modified by doping, or by the application of electrical fields or light, devices made from semiconductors can be used for amplification, switching, and energy conversion.

Semiconductors in their natural state are poor conductors because a current requires the flow of electrons, and semiconductors have their valence bands filled, preventing the entire flow of new electrons. Several developed techniques allow semiconducting materials to behave like conducting materials, such as doping or gating. These modifications have two outcomes: *n*-type and *p*-type. These refer to the excess or shortage of electrons, respectively. An unbalanced number of electrons would cause a current to flow through the material.

Some of the properties of semiconductor materials were observed throughout the mid-19th and first decades of the 20th century. The first practical application of semiconductors in electronics was the 1904 development of the cat's-whisker detector, a primitive semiconductor diode used in early radio receivers. Developments in quantum physics led in turn to the invention of the transistor in 1947, the integrated circuit in 1958, and the MOSFET (Metal–Oxide–Semiconductor Field-Effect Transistor) in 1959.

The most common semiconducting materials are crystalline solids, but amorphous and liquid semiconductors are also known. These include hydrogenated amorphous silicon and mixtures of arsenic, selenium, and tellurium in a variety of proportions. These compounds share with better-known semiconductors the properties of intermediate conductivity and a rapid variation of conductivity with temperature, as well as occasional negative resistance. Such disordered materials lack the rigid crystalline structure of conventional semiconductors such as silicon. They have generally used in thin film structures, which do not require material of higher electronic quality, being relatively insensitive to impurities and radiation damage.

6.5 CLASSIFICATIONS OF SEMICONDUCTORS

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This text focuses on the semiconductors and their properties. Most widely used semiconductors are Silicon (Si), Germanium (Ge), Selenium (Se) etc., that exists as simple semiconductors and compound semiconductors such as Gallium Arsenide (GaAs), Indium Phosphate (InP), Gallium Nitride (GaN) etc. Semiconductors based on the purity of the materials are classified as

- Intrinsic Semiconductors
- Extrinsic semiconductors

6.5.1 Intrinsic Semiconductors

Semiconductors that exists in pure form without any impurities added are called as intrinsic semiconductors. Consider the semiconductor Silicon, Si with atomic number 14. It has 14 number of protons and 14 number of electrons. The first shell occupies 2 electrons, the second shell occupies 8 electrons and the third shell which could accommodate 18 electrons has only 4 valence electrons. Similarly, germanium with an atomic number of 32 as shown in Figure 6.3a has 4 shells with an outermost shell consisting of 4 valence electrons. These atoms exist in the crystalline structure with bonding as shown in Figure 1.5b. One atom of silicon shares the bonding with 4 other atoms thereby filling the 3rd shell of an atom with all 8 electrons creating a stable composition of silicon crystal. This type of bonding is known as covalent bonding.

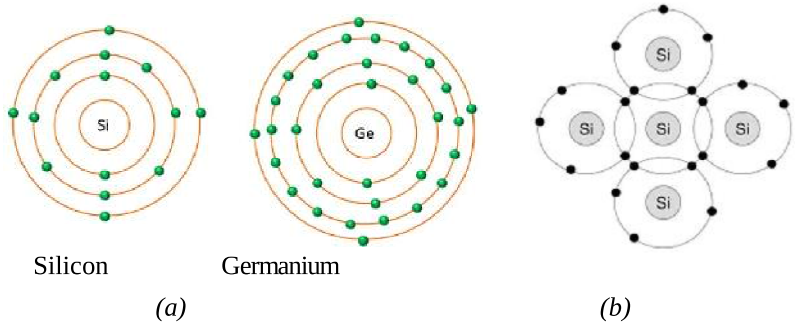


Fig. 6.3 *(a)Atomic Structure of Silicon and Germanium, (b) Crystalline Structure of Silicon*

Intrinsic semiconductors behave as perfect insulators under normal room temperatures. Silicon and germanium that consists of 4 valence electrons in their outermost shells are also known as **tetravalent atoms**. Similarly, atoms with three valence electrons are known as **trivalent atoms** and atoms with five valence electrons are known as **pentavalent atoms**.

Conduction in Intrinsic Semiconductors

When an external energy is supplied to the intrinsic semiconductor crystal, the electrons absorb the energy supplied and gain enough energy to break the covalent bond and are set free to move as free electrons in the crystal. Such free electrons move randomly inside the crystal until they lose their energy and finds a bonding pair of an electron with some other atom. When the electron leaves a covalent bond due to external energy, they leave behind a vacant space known as holes. Electrons are negatively charged and the vacant hole spaces wanting for electrons to occupy the space are considered as positively charged. When the free electrons leave the covalent bonding due to external energy, they form an electron-hole pair.

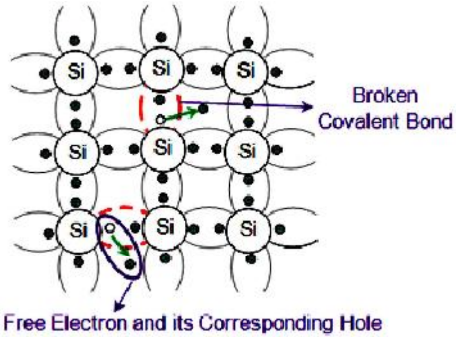


Fig. 6.4 *Conduction Inside Intrinsic Semiconductors*

Electron Current and Hole Current

Current constituted by electrons inside the semiconductor crystal are called an **electron current**. Since electrons are negatively charged, when a potential is applied across the semiconductor crystal, the electrons are attracted towards the positive terminal of the battery.

Current constituted by holes inside a semiconductor crystal are known as **hole current**. Though the holes (vacant spaces) do not move, consequent movement of electrons creates an illusion such that holes move, but in the opposite direction as that of the electron. Electron movement occurs towards the positive polarity of the battery and the hole movement is illusioned to appear as though holes move towards negative terminal of the battery. The movement of holes, i.e., the movement towards a negative terminal (from the positive terminal) is considered as the conventional current movement and hence the hole movement is considered as conventional current flow and the electron movement is considered as the electron flow. The electron and hole current is depicted in Figure 6.5

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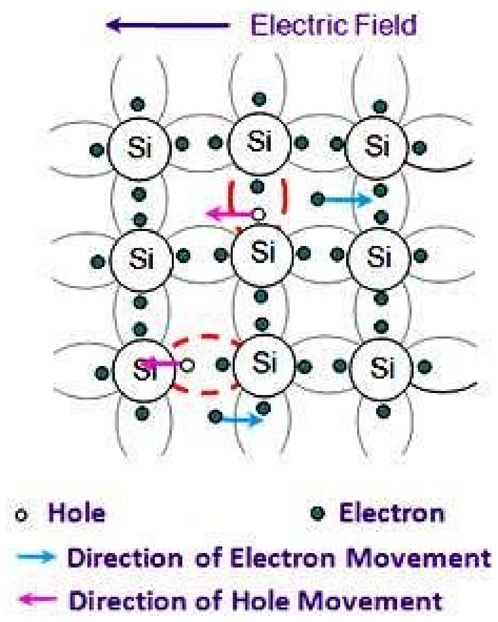


Fig. 6.5 *Electron and Hole Current*

The hole current is known as the conventional current is opposite to the direction of the electron movement and flows from the positive terminal of the battery to the negative terminal of the battery. The electron current and hole current occur due to two process, they are

- Drift and
- Diffusion.

Drift Current

The current flow that takes place due to the application of the external potential through a battery results in drifting of the electrons, thereby resulting in drift current. When an external energy is applied to the semiconductor crystal, the electrons gain energy and starts to drift across the crystal and tends move towards the battery terminal (positive terminal). Such currents are said to be drift current caused due to drifting of electrons.

Diffusion Current

Diffusion current occurs due to the movement of electrons through diffusion when they move from higher concentration area to a lower concentration area of the semiconductor crystal without applying any external force or energy.

6.5.2 Extrinsic Semiconductors

An extrinsic semiconductor is one that has been doped, i.e., during manufacture of the semiconductor crystal a trace element or chemical called a doping agent has been incorporated chemically into the crystal, for the purpose of giving it different

electrical properties than the pure semiconductor crystal, which is called an intrinsic semiconductor. In an extrinsic semiconductor, these foreign dopant atoms in the crystal lattice provide the charge carriers which carry electric current through the crystal. The doping agents used are of two types, resulting in two types of extrinsic semiconductor. An electron donor dopant is an atom which, when incorporated in the crystal, releases a mobile conduction electron into the crystal lattice. An extrinsic semiconductor which has been doped with electron donor atoms is called an *n*-type semiconductor, because the majority of charge carriers in the crystal are negative electrons. An electron acceptor dopant is an atom which accepts an electron from the lattice, creating a vacancy where an electron should be called a hole which can move through the crystal like a positively charged particle. An extrinsic semiconductor which has been doped with electron acceptor atoms is called a *p*-type semiconductor, because the majority of charge carriers in the crystal are positive holes.

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Doping is the key to the extraordinarily wide range of electrical behaviour that semiconductors can exhibit, and extrinsic semiconductors are specifically used to make semiconductor electronic devices, such as diodes, transistors, integrated circuits, semiconductor lasers, LEDs, and photovoltaic cells. Sophisticated semiconductor fabrication processes like photolithography can implant different dopant elements in different regions of the same semiconductor crystal wafer, creating semiconductor devices on the wafer's surface. For example a common type of transistor, the *n-p-n* bipolar transistor, consists of an extrinsic semiconductor crystal with two regions of *n*-type semiconductor, separated by a region of *p*-type semiconductor with metal contacts attached to each part.

Intrinsic semiconductors are the purest form of semiconductors. Their conductivity of electricity is limited. They have an equal number of electrons and holes. To make semiconductors practically relevant with better conduction of current, it is important to enhance the conduction capability of semiconductors. One such technique to enhance the conductivity is by the process of **doping**. Doping is a process of adding impurities to the intrinsic semiconductors, such that the conductivity of the semiconductors is improved. The impurity that is added to the semiconductor is called as a dopant. The doped semiconductors are called as extrinsic semiconductors. The type of impurities added may enhance the number of electrons or they may enhance the number of holes. Hence, depending on the type of impurities, the extrinsic semiconductors can be classified as

- *n*-type semiconductors
- *p*-type semiconductors.

When an intrinsic semiconductor is added with an impurity with pentavalent atoms, *n*-type semiconductors are formed. When an intrinsic semiconductor is added with a trivalent impurity atom, *p*-type semiconductors are formed. Pentavalent impurity atoms are also known as donor atoms and trivalent atoms

are known as acceptor atoms. Atoms that donate atoms to the host atoms are called donor atoms and the atoms that accept an electron from the host atoms are called acceptor atoms.

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n-Type Semiconductor

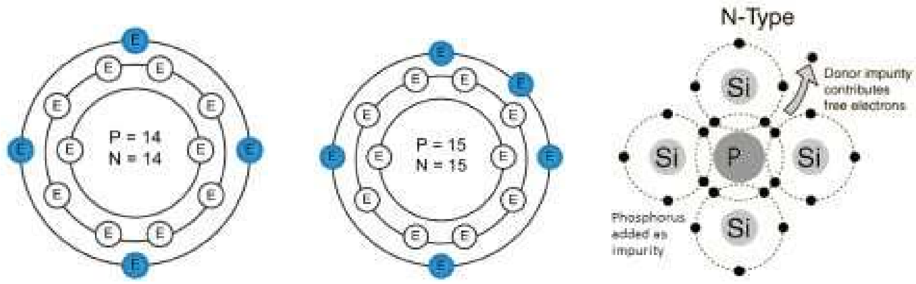


Fig. 6.6 *n-Type Semiconductor*

When a pentavalent impurity atom from group V of the periodic table such as Phosphorus (P) or Arsenic (As) is added to the intrinsic silicon atom, *n*-type semiconductors are formed.

When the *n*-type impurity atom (donor atoms) is added with the intrinsic silicon atom, the four valence electrons out of five valence electrons in the impurity atom forms a covalent bond with the four silicon atoms as shown in Figure 1.8. The remaining one valence electrons from the impurity atoms remain as free electron inside the mixture crystal. Similarly, when 1 of phosphorus can generated free electrons of the order of   number of free electrons. Number of free electrons required are controlled by the amount of pentavalent impurity added to the intrinsic silicon atom.

The Conductivity of *n*-Type Semiconductors

The mobility of electrons is approximately three times that of the mobility of holes. When more free electrons are added to the intrinsic semiconductor, the average energy level of the semiconductor increases. This makes the electrons move easier from the valence band to the conduction band even with an application of the small amount of an external potential. In addition, the Fermi level, which marks the energy level of electrons is closer to the conduction band as shown in Figure 6.7. In *n*-type semiconductors since the electrons are more than the number of holes, electrons are known as majority carriers and the holes are known as minority carriers. The current constituted by majority carriers (electrons) are predominant and the current constituted by minority carriers (holes) are negligent.

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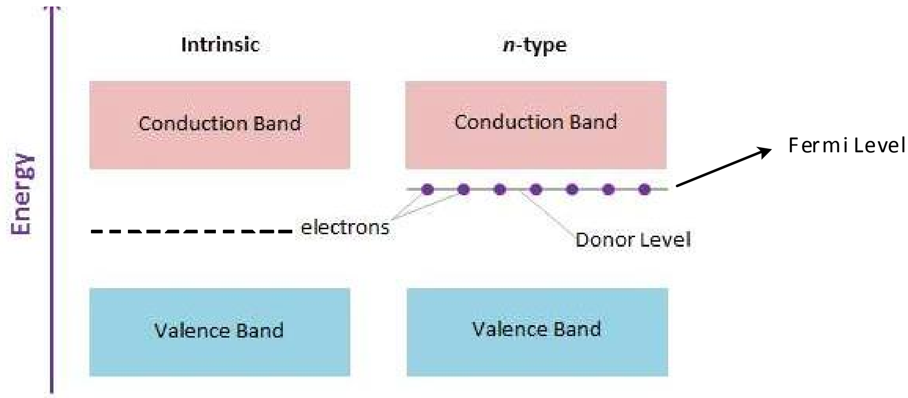


Fig. 6.7 *n-Type Semiconductor Band Diagram*

p-Type Semiconductors

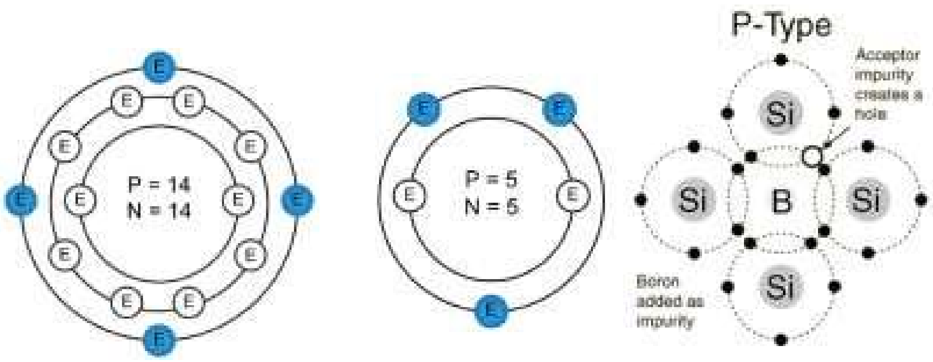


Fig. 6.8 *p-Type Semiconductor*

When a trivalent impurity atom from group III of the periodic table such as Boron (B) or Gallium (Ga) is added to the intrinsic silicon atom, *p*-type semiconductors are formed.

When the p-type impurity atom (acceptor atoms) is added with the intrinsic silicon atom, the three valence electrons of the acceptor atoms form a covalent bond with the three silicon atoms leaving behind one silicon atom form an electron-hole pair as shown in Figure 6.8. The one hole generated due to nonavailability of an electron to fill from the impurity atom forms one electron-hole pair. Similarly, when 1 of Boron can generated electron-hole pairs of the order of numba er of holes. Number of holes required are controlled by the amount of trivalent impurity added to the intrinsic silicon atom.

The Conductivity of *p*-Type Semiconductors

When more holes are added to the intrinsic semiconductor, the average energy level of the semiconductor decreases. Hence, a larger magnitude of external energy needs to be applied to make the electrons conduct. In other words to make the electrons move from the valence band to conduction band. However, it is easier

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to make the electrons conduct in the reverse direction by applying a negative potential. The Fermi level, which marks the energy level of electrons is closer to the valence band as shown in Figure 6.9. In *p*-type semiconductors since the holes are more than the number of electrons, holes are known as majority carriers in *p*-type semiconductors and the electrons are known as minority carriers. The current constituted by majority carriers (holes) are predominant and the current constituted by minority carriers (electrons) are negligent.

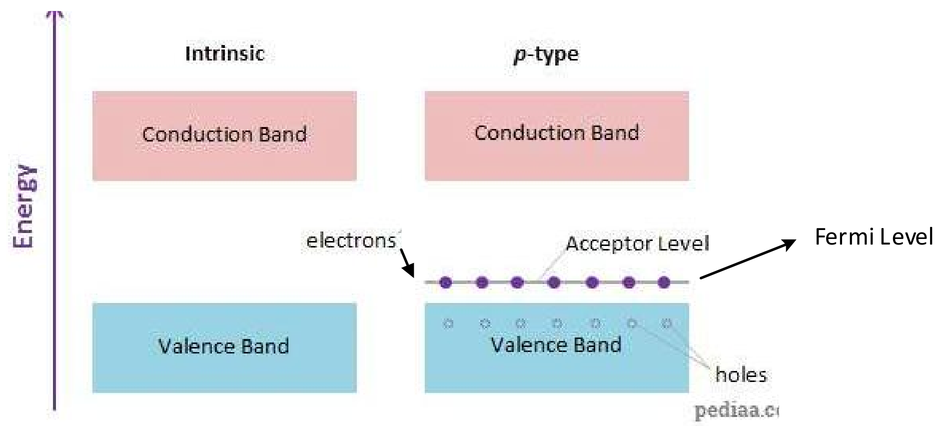


Fig. 6.9 *p-Type Semiconductor Band Diagram*

p-n Junction Diode

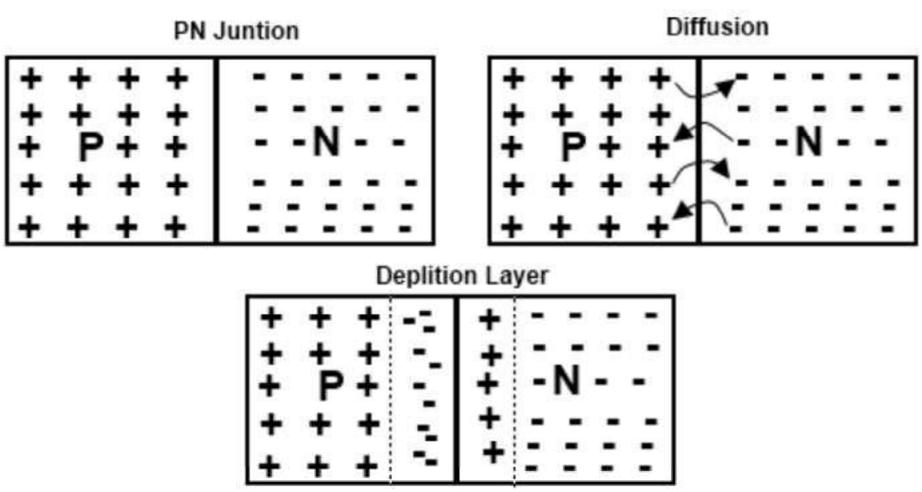


Fig. 6.10 *p-n Diffusion*

When a *p*-type semiconductor and *n*-type semiconductor are joined together, diffusion takes place. Since the *p*-type material is highly concentrated with holes leading to an overall high positive charge material and *n*-type a negatively charged material due to the concentration of electrons, when joined together, they together generate a high potential on the *p*-type side and now potential on the *n*-type side. This leads to the process of diffusion making the electrons to move towards the *p*-

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side. As electrons move towards the *p*-type crossing the junction, they leave behind holes. The electrons spend enough energy to cross over the junction after which they occupy a hole position nearer to the junction. Thus, holes are formed on the *n*-type side of the junction and electrons on the *p*-type junction. Any electron that wants to cross over the junction further must have enough energy to overcome the holes and the junction together. Thus, creates a region of depletion of charges with positive charges on *n*-type and negative charges on *p*-type. The buildup of the depletion region continues until the electrons cannot diffuse further. Once the diffusion stops, the potential difference created by the process of electron diffusion results in approximately 0.7 volts for silicon semiconductors and 0.3 volts for germanium semiconductors. This potential difference created by the process of diffusion is also known as barrier potential. The electrons that require moving to the *p*-type material further must overcome the barrier potential of 0.7V for silicon material. The electrons alone do not possess such amount of energy to cross the barrier potential and hence on the application of an external voltage equal to the barrier potential is required to make the electrons move to the other side of the *p*-*n* junction.

The barrier potential depends on various factors as follows:

- Type of semiconductor
- Type of impurity
- External atmospheric temperature and
- The concentration of intrinsic semiconductor

6.6 FERMI ENERGIES OF IMPURITY SEMICONDUCTORS

In an extrinsic semiconductor, the number of electrons in the conduction and the number of holes in the valence band are not equal. Henceforth, the chances of the occupation of the energy levels in valance and conduction bands are not equal. Therefore, in the case of extrinsic semiconductors, the Fermi level lies close to any of the valance or conduction band.

In semiconductors, the Fermi level is inside a band gap; however, in semiconductors the bands are near enough to the Fermi level to be thermally populated with electrons or holes. As we know that electrical conductivity arises due to the presence of electrons in states that are delocalized (extending through the material), however in order to transport electrons a state must be partially filled, containing an electron only part of the time. If the state is always occupied with an electron, then it is inert, blocking the passage of other electrons via that state. The energies of these quantum states are critical since a state is partially filled only if its energy is near the Fermi level.

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High conductivity in material comes from it having many partially filled states and much state delocalization. Metals are good electrical conductors and have many partially filled states with energies near their Fermi level. Insulators, by contrast, have few partially filled states, their Fermi levels sit within band gaps with few energy states to occupy. Importantly, an insulator can be made to conduct by increasing its temperature: heating provides energy to promote some electrons across the band gap, inducing partially filled states in both the band of states beneath the band gap (valence band) and the band of states above the band gap (conduction band). An (intrinsic) semiconductor has a band gap that is smaller than that of an insulator and at room temperature, significant numbers of electrons can be excited to cross the band gap.

Some wider-band gap semiconductor materials are sometimes referred to as semi-insulators. When undoped, these have electrical conductivity nearer to that of electrical insulators, however they can be doped (making them as useful as semiconductors). Semi-insulators find niche applications in micro-electronics, such as substrates for HEMT (High-Electron-Mobility Transistor). An example of a common semi-insulator is gallium arsenide. Some materials, such as titanium dioxide, can even be used as insulating materials for some applications, while being treated as wide-gap semiconductors for other applications.

In an *n*-type semiconductor, the Fermi level is greater than that of the intrinsic semiconductor and lies closer to the conduction band than the valence band whereas for *p*-type semiconductors, the Fermi level is below the intrinsic semiconductor and lies closer to the valence band than the conduction band.

Extrinsic semiconductors are formed by adding suitable **impurities** to the intrinsic semiconductor. The added impurity is very small, of the order of one atom per million atoms of the pure semiconductor. The added impurity may be pentavalent or trivalent. Depending on the type of impurity added, the extrinsic semiconductors can be divided into two classes: *n*-type and *p*-type.

Fermi Level in *n*-Type Semiconductor

When **pentavalent impurity** is added to pure semiconductor, it results in *n*-type semiconductor. The fifth electron of donor atom is loosely bounded. By small thermal energy or by applying electric field, this electron can be easily excited from the valence band to the conduction band. So donor donates free electrons. Since current carriers are negatively charged particles, this type of semiconductor is called *n*-type semiconductor.

A pentavalent impurity is substituted in order to obtain an *n*-type semiconductor. Each pentavalent impurity contributes an extra electron. In this way, the presence of pentavalent impurity leaves free electrons in the conduction band.

In such a case, the number of electrons present in the conduction band is more than the number of holes present in the valence band, at room temperature. Henceforth, the chances of occupation of energy levels in the conduction band by the electrons are more than the chances of occupation of energy levels by the holes in the valence band. This probability of occupation of energy levels is represented in terms of Fermi energy level. Therefore, the Fermi level in the n-type semiconductor lies close to the conduction band.

The Fermi level for an *n*-type semiconductor can be written as

Where EF is the Fermi level and KB is the Boltzmann constant. T is the temperature in Kelvin. EC is the energy of the conduction band. NC defines the effective density of states of the conduction band, whereas, ND is the donor atom concentration in the extrinsic semiconductor.

Fermi Level in *p*-Type Semiconductor

When **trivalent impurity** is added to pure semiconductor, it results in *p*-type semiconductor. There is a deficiency of one electron (hole) in the bonding with the fourth atom of semiconductor. Due to this, a hole is created in the adjacent atom. Since current carriers are positively charged particles, this type of semiconductor is called *p*-type semiconductor.

In the case of a *p*-type semiconductor, trivalent impurities are added to the intrinsic semiconductor. Each trivalent impurity generates a hole in the valence band. The hole is receptive towards an electron. In this way, trivalent impurities create a proportional number of holes in the valence band.

In this scenario, at room temperature, the counting of holes in the valence band is greater than the count of electrons available in the conduction band. Therefore, the chances of occupation of energy levels in the valence band by the holes are more than the chances of the conduction band to be occupied by the electrons. The probability of the occupation of energy levels is characterized in terms of Fermi level. Henceforth, in the *p*-type semiconductors, the Fermi level lies close to the valence band.

In a *p*-type semiconductor, the Fermi level can be explained as

Where EF is the Fermi level and KB is the Boltzmann constant. T is the temperature in Kelvin. EV is the energy of conduction band. Moreover, NV is the effective density of states of the valence band and NA defines the concentration of acceptor atoms.

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Check Your Progress

1. Explain the band theory of solids.
2. Define the band structure in solids.
3. Elaborate on the Kronig-Penney model.
4. What do you understand by the semiconductors?
5. Elucidate on the classifications of semiconductors.
6. Define the intrinsic semiconductors.
7. Explain the electron current and hole current.
8. What do you mean by the diffusion current?
9. Interpret the extrinsic semiconductors.
10. State the Fermi energies of impurity semiconductors.

6.7 ANSWERS TO CHECK YOUR PROGRESS QUESTIONS

1. In the case of a single isolated atom, the electrons in any orbit have a definite energy. As a result, they occupy discrete energy levels. The Pauli exclusion principle allows each energy level to contain only two electrons.
2. The electrons in any orbit of atom within a solid can have a range of energies rather than a single value. Thus, the range of energies possessed by an electron in a solid is known as energy band. i.e., each energy level of an isolated atom becomes a band in a solid.
3. The Kronig–Penney model (named after Ralph Kronig and William Penney) is a simple, idealized quantum-mechanical system that consists of an infinite periodic array of rectangular potential barriers.
4. Semiconductors are defined by their unique electric conductive behaviour, somewhere between that of a conductor and an insulator. A semiconductor material has an electrical conductivity value falling between that of a conductor, such as metallic copper, and an insulator, such as glass.
5. Semiconductors based on the purity of the materials are classified as: Intrinsic Semiconductors, and Extrinsic semiconductors.
6. Semiconductors that exists in pure form without any impurities added are called as intrinsic semiconductors. Consider the semiconductor Silicon, Si with atomic number 14.
7. Current constituted by electrons inside the semiconductor crystal are called an electron current, while current constituted by holes inside a semiconductor crystal are known as hole current.

8. Diffusion current occurs due to the movement of electrons through diffusion when they move from higher concentration area to a lower concentration area of the semiconductor crystal without applying any external force or energy.
9. An extrinsic semiconductor is one that has been doped, i.e., during manufacture of the semiconductor crystal a trace element or chemical called a doping agent has been incorporated chemically into the crystal, for the purpose of giving it different electrical properties than the pure semiconductor crystal, which is called an intrinsic semiconductor.
10. In semiconductors, the Fermi level is inside a band gap; however, in semiconductors the bands are near enough to the Fermi level to be thermally populated with electrons or holes.

6.8 SUMMARY

- In the case of a single isolated atom, the electrons in any orbit have a definite energy. As a result, they occupy discrete energy levels. The Pauli exclusion principle allows each energy level to contain only two electrons.
- The electrons in any orbit of atom within a solid can have a range of energies rather than a single value. Thus, the range of energies possessed by an electron in a solid is known as energy band. i.e., each energy level of an isolated atom becomes a band in a solid.
- The Kronig–Penney model (named after Ralph Kronig and William Penney) is a simple, idealized quantum-mechanical system that consists of an infinite periodic array of rectangular potential barriers.
- Semiconductors are defined by their unique electric conductive behaviour, somewhere between that of a conductor and an insulator. A semiconductor material has an electrical conductivity value falling between that of a conductor, such as metallic copper, and an insulator, such as glass.
- Semiconductors based on the purity of the materials are classified as: Intrinsic Semiconductors, and Extrinsic semiconductors.
- Semiconductors that exists in pure form without any impurities added are called as intrinsic semiconductors. Consider the semiconductor Silicon, Si with atomic number 14.
- Current constituted by electrons inside the semiconductor crystal are called an electron current, while current constituted by holes inside a semiconductor crystal are known as hole current.

NOTES

- Diffusion current occurs due to the movement of electrons through diffusion when they move from higher concentration area to a lower concentration area of the semiconductor crystal without applying any external force or energy.
- An extrinsic semiconductor is one that has been doped, i.e., during manufacture of the semiconductor crystal a trace element or chemical called a doping agent has been incorporated chemically into the crystal, for the purpose of giving it different electrical properties than the pure semiconductor crystal, which is called an intrinsic semiconductor.
- In semiconductors, the Fermi level is inside a band gap; however, in semiconductors the bands are near enough to the Fermi level to be thermally populated with electrons or holes.
- Extrinsic semiconductors are formed by adding suitable impurities to the intrinsic semiconductor. The added impurity is very small, of the order of one atom per million atoms of the pure semiconductor. The added impurity may be pentavalent or trivalent. Depending on the type of impurity added, the extrinsic semiconductors can be divided into two classes: *n*-type and *p*-type.

6.9 KEY WORDS

- **Semiconductors:** Semiconductors are defined by their unique electric conductive behaviour, somewhere between that of a conductor and an insulator. A semiconductor material has an electrical conductivity value falling between that of a conductor, such as metallic copper, and an insulator, such as glass.
- **Intrinsic semiconductors:** Semiconductors that exists in pure form without any impurities added are called as intrinsic semiconductors. Consider the semiconductor Silicon, Si with atomic number 14.
- **Drift current:** The current flow that takes place due to the application of the external potential through a battery results in drifting of the electrons, thereby resulting in drift current.
- **Diffusion current:** Diffusion current occurs due to the movement of electrons through diffusion when they move from higher concentration area to a lower concentration area of the semiconductor crystal without applying any external force or energy.
- **Extrinsic semiconductors:** An extrinsic semiconductor is one that has been doped, i.e., during manufacture of the semiconductor crystal a trace element or chemical called a doping agent has been incorporated chemically into the crystal.

- ***n*-type semiconductors:** When a pentavalent impurity atom from group V of the periodic table such as Phosphorus (P) or Arsenic (As) is added to the intrinsic silicon atom, *n*-type semiconductors are formed.
- ***p*-type semiconductors:** When a trivalent impurity atom from Group III of the periodic table such as Boron (B) or Gallium (Ga) is added to the intrinsic silicon atom, *p*-type semiconductors are formed.

NOTES

6.10 SELF ASSESSMENT QUESTIONS AND EXERCISES

Short-Answer Questions

1. Define the band theory of solids.
2. Elaborate on the band structure in solids.
3. State the Kronig-Penney model.
4. What do you mean by the semiconductors?
5. Interpret the classifications of semiconductors.
6. Explain the intrinsic semiconductors.
7. Define the electron current and hole current.
8. What do you understand by the diffusion current?
9. Elucidate on the extrinsic semiconductors.
10. Explain the Fermi energies of impurity semiconductors.

Long-Answer Questions

1. Discuss briefly the band theory of solids with the help of examples.
2. Analyse the Kronig-Penney model giving examples.
3. Explain about the semiconductors giving appropriate examples.
4. Describe the classifications of semiconductors.
5. Briefly explain the Fermi energies of impurity semiconductors.

6.11 FURTHER READINGS

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UNIT 7 DIELECTRIC PROPERTIES OF MATERIALS

NOTES

Structure

7.0 Introduction
7.1 Objectives
7.2 Polarization
7.3 Local Electric Field
7.4 Clausius-Mossotti Relation
7.5 Polarization Field
7.6 Lorentz Field
7.7 Answers to Check Your Progress Questions
7.8 Summary
7.9 Key Words
7.10 Self Assessment Questions and Exercises
7.11 Further Readings

7.0 INTRODUCTION

The term dielectric was created by William Whewell in response to a request from Michael Faraday. A perfect dielectric is a material with zero electrical conductivity (perfect conductor infinite electrical conductivity), thus exhibiting only a displacement current; therefore it stores and returns electrical energy as if it were an ideal capacitor.

A dielectric (or dielectric material) is an electrical insulator that can be polarized by an applied electric field. When a dielectric material is placed in an electric field, electric charges do not flow through the material as they do in an electrical conductor, but instead only slightly shift from their average equilibrium positions, causing dielectric polarization.

Dielectric materials are the materials with a high polarizability. The latter is expressed by a number called the relative permittivity. The term insulator is generally used to indicate electrical obstruction while the term dielectric is used to indicate the energy storing capacity of the material (by means of polarization). A common example of a dielectric is the electrically insulating material between the metallic plates of a capacitor. The polarization of the dielectric by the applied electric field increases the capacitor's surface charge for the given electric field strength.

Dielectric materials can be solids, liquids, or gases. A high vacuum can also be a useful, nearly lossless dielectric even though its relative dielectric constant is only unity. Solid dielectrics are perhaps the most commonly used dielectrics in electrical engineering, and many solids are very good insulators. Some examples include porcelain, glass, and most plastics. Air, nitrogen and sulphur hexafluoride are the three most commonly used gaseous dielectrics. Because dielectrics resist the flow of electricity, the surface of a dielectric may retain stranded excess electrical charges. This may occur accidentally when the dielectric is rubbed (the triboelectric effect).

Some dielectrics can generate a potential difference when subjected to mechanical stress, or (equivalently) change physical shape if an external voltage is applied across the material. This property is called piezoelectricity. Piezoelectric materials are another class of very useful dielectrics.

In this unit, you will study about the polarisation, local electric field, the Clausius–Mossotti relation, polarization field, and the Lorentz field.

7.1 OBJECTIVES

After going through this unit, you will be able to:

- Understand the basics of polarisation
- Explain the local electric field
- Elaborate on the Clausius-Mossotti relation
- Comprehend on the polarisation field
- Analyse the Lorentz field

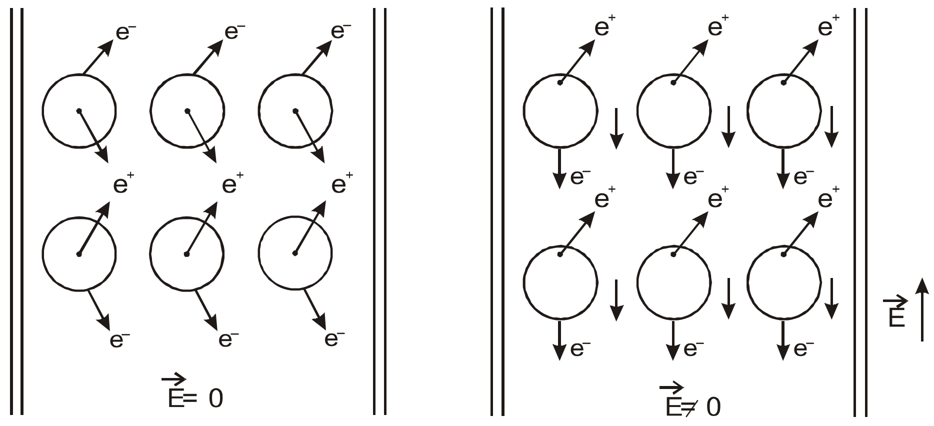
7.2 POLARIZATION

The behaviour of a dielectric material can be changed by the application of an external electric field.

We know that, in an atom there is a positively charged nucleus at the centre surrounded by orbiting electrons (electron cloud) which are negatively charged. An isolated atom does not have any dipole moment; since, the centeroid of the negative charge distribution and the positive charge coincide.

But, when an external electric field is applied, it causes the electron cloud to move in opposite direction. Thus, the centeroids of the positive and negative charges now no longer coincide and as a result an electric dipole is induced in the atom. Thus, the atoms are said to be polarised. The Figure 7.1 illustrates the above process.

NOTES



No polarisation
Centroids of positive and negative charge coincide

Polarisation
Non coincidence of centroids of positve and negative charge.

Fig. 7.1 *Dielectric Polarisation*

Note:
- **Dipole :** A pair of equal and opposite charges separated by a small distance constitutes an electric dipole.
- The product of magnitude of one of the charges q and the distance of their separation *x* is called the dipole moment μ, i.e., $\mu = q \times x$.

Therefore, polarisation is defined as the process of creating or inducing dipoles in a dielectric material by an external electric field. The polarisation increases with the field upto the critical value.

On the basis of polarisation concept, *the dielectrics are the materials that have either permanent dipoles or induced dipoles in the presence of an applied electric field.* They are classified into two categories, namely *polar and non-polar dielectrics.*

Non-Polar Dielectrics

A dielectric material in which, there is no permanent dipole existence in the absence of an external field is called non-polar dielectrics.

This is because, in these type of dielectrics, the centroid of the positive and negative charges of the molecules constituting the dielectric material coincide. ***Examples*** *are* H_2, N_2, O_2, CO_2 and CH_4. These molecules are called *non-polar molecules.*

Polar Dielectrics

A dielectric material in which there is an existence of permanent dipole even in the absence of an external field is called a polar dielectric.

This is because, in these type of dielectrics, the center of the positive charges and negative charges of the molecules constituting the dielectric material do not coincide even in the absence of an external field.

NOTES

***Examples** are* H_2O, HCl and CO. These molecules are called *polar molecules.*

7.3 LOCAL ELECTRIC FIELD

The electric field acting at an atom in a dielectric known as the internal field or local field E_{int} is different from the applied external field.

The internal field, or the local field, is the electric field acting at an atom of a solid or liquid dielectric subjected to an external field. It is the resultant of the applied field and the field due to all the surrounding dipoles.

Calculation of the Internal Field (Local Field)

The following method suggested by Lorentz is used to establish the relation between the applied field E and the internal field E_{int}.

The given dielectric is placed in between a parallel plate capacitor and is uniformly polarised by applying an external field E.

To evaluate E_{int}, we must calculate the total field acting on an atom A (dipole) within the dielectric. For this to calculate, imagine a spherical cavity (Lorentz sphere) around the atom A (dipole) inside the dielectric as shown in Figure 7.2. Further, it is assumed that, the radius r of the cavity is large compared to the radius of the atom. The medium lying external to the cavity is treated as a continuous medium as for as the atom A is concerned.

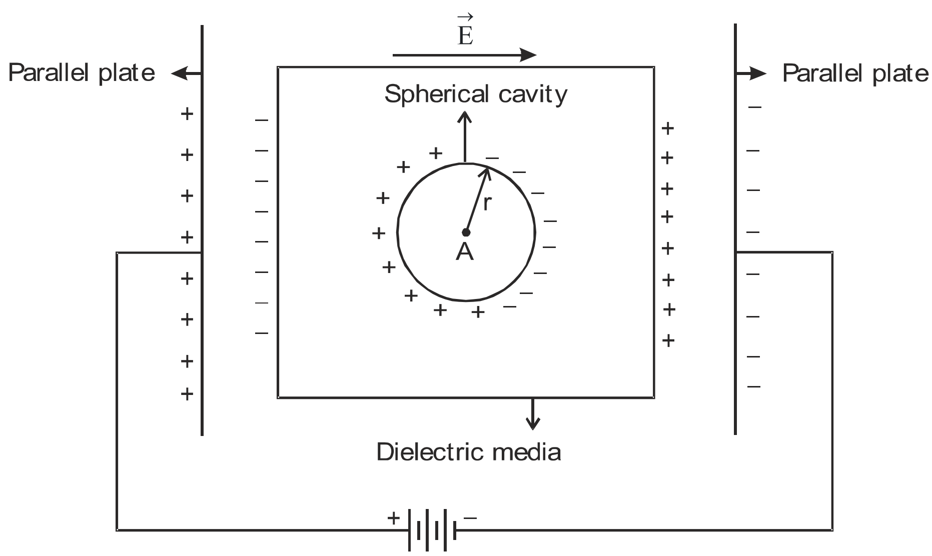


***Fig. 7.2** Calculation of Internal Field for a Cubic Structure*

The interaction of the atom A (dipole) with other dipoles within the cavity is treated microscopically; since, the medium very close to the atom A (dipole) within the cavity is considered to be discrete.

The internal field or local field, acting on the central atom (dipole) is thus given by

$$E_{int} = E_1 + E_2 + E_3 + E_4 \qquad ...(7.1)$$

Where

E_1 is the field due to the charges on the plates.

E_2 is the field due to the polarising charges lying at the external surface of the dielectric medium. *This is also known as the depolarisation field.*

E_3 is the field due to the polarisation charges lying on the surface of the sphere which is *known as the Lorentz field.*

E_4 is the field due to other dipoles lying within the sphere.

To Find E_1, E_2, E_3 and E_4 Values

Field E_1

When a dielectric medium is polarised due to an electric field E, the displacement vector D is given by

$$D = \varepsilon_o E + P \qquad ...(7.2)$$

From field theory, the field at A due to the charge density on the plates is given by,

$$D = \varepsilon_o E_1 \qquad ...(7.3)$$

Therefore, the equating equations (7.2) and (7.3), we get

$$\varepsilon_o E_1 = \varepsilon_o E + P$$

Dividing the above equation by ε_o, we get

$$E_1 = E + \frac{P}{\varepsilon_o} \qquad ...(7.4)$$

Field E_2

E_2 is the field due to the polarisation charges on the external surface of the dielectric. This field acts in a direction opposite to the external field. Therefore, it is given by

$$E_2 = \frac{-P}{\varepsilon_o} \qquad ...(7.5)$$

Field E_3

E_3 is the field due to polarisation charges on the surface of the cavity. This field value is evaluated as follows.

NOTES

Consider an enlarged view of the cavity as shown in figure 7.3. In order to calculate this field acting on the atom A in the direction of the field consider an elemental ring EFGH perpendicular to the field direction. The area of the ring shaped element along the surface of the sphere is given by

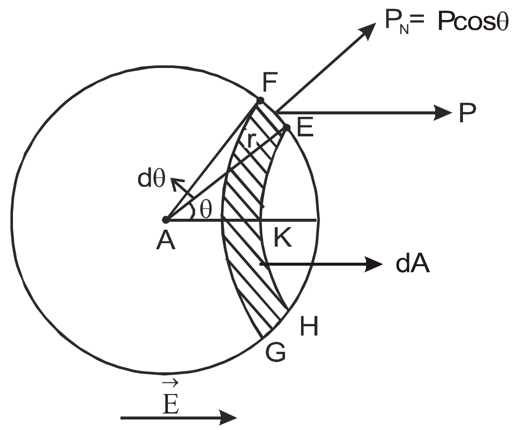


Fig. 7.3 *Lorentz Field*

$$dA = 2\pi \times EK \times EF$$
$$= 2\pi \times r\sin\theta \times rd\theta$$

[where EF = rdθ is the arc length. From the figure, $\sin\theta = \frac{EK}{r}$. Therefore, EK = rsinθ].

Hence, $$dA = 2\pi r^2 \sin\theta d\theta \quad ...(7.6)$$

From the definition of polarisation, (defined as the induced surface charge per unit area, i.e., $P = \frac{q}{A}$) the charge q on dA is equal to the product of the normal component of polarisation and surface area.

i.e., $$q = P_N \cdot dA$$

The polarisation P is parallel to E. Its component normal to dA is $P_N = P\cos\theta$.

∴ $$q = P\cos\theta \, dA \quad ...(7.7)$$

Substituting for dA from Equations (7.6) in (7.7)

$$q = P\cos\theta.\ 2\pi r^2 \sin\theta \, d\theta \quad ...(7.8)$$

Thus, the electric field dE_3 at A due to the charge q is given by (Coulomb's law)

$$dE_3 = \frac{q}{4\pi\varepsilon_o r^2}$$

Substituting for q from Equation (7.8) in the above,

NOTES

$$dE_3 = \frac{P\cos\theta . 2\pi r^2 \sin\theta d\theta}{4\pi\varepsilon_o r^2}$$

$$= \frac{P\cos\theta \sin\theta d\theta}{2\varepsilon_o} \quad ...(7.9)$$

The above field is having two components, one component (cosθ) along the applied field and the other component (sinθ) perpendicular to the field E.

The field at A due to the perpendicular component is zero. Since, the components are symmetrically distributed around the axis, they will cancel out each other.

Thus, the component of field along the applied field direction is

$$dE_3 = \frac{P\cos\theta \sin\theta d\theta}{2\varepsilon_o} \times \cos\theta$$

or

$$dE_3 = \frac{P\cos^2\theta \sin\theta d\theta}{2\varepsilon_o} \quad ...(7.10)$$

Therefore, the field at A due to the surface charge on the cavity is obtained by integrating over the whole surface of the sphere.

i.e.,

$$E_3 = \frac{P}{2\varepsilon_o} \int_o^{\pi} \cos^2\theta \sin\theta d\theta$$

$$= \frac{P}{2\varepsilon_o} . \frac{2}{3}$$

$$= \frac{P}{3\varepsilon_o} \quad \left[\because \int_0^{\pi} \cos^2\theta \sin\theta \, d\theta = 2/3 \right]$$

$$\therefore \quad \mathbf{E_3 = \frac{P}{3\varepsilon_o}} \quad ...(7.11)$$

Note:

To prove $\int_o^{\pi} \cos^2\theta \sin\theta d\theta = \frac{2}{3}$.

Proof: Let $x = \cos\theta$

$\therefore \quad dx = -\sin\theta d\theta$

When $\theta = 0 \quad x = 1$

$\theta = \pi \quad x = -1$

$$\therefore \quad \int_o^{\pi} \cos^2\theta \sin\theta d\theta = -\int_1^{-1} x^2 dx$$

NOTES

$$= \int_{-1}^{1} x^2 dx$$

$$= \left.\frac{x^3}{3}\right]_{-1}^{+1} = \frac{2}{3}.$$

Field E_4

This is the field due to the dipoles within the cavity which depends on the crystal structure.

This field E_4 is zero for a spherically symmetric system i.e., for a cubic structure. Hence, assuming the dielectric material to be of a cubic structure, E_4 is taken to be zero in this calculation.

i.e., for a cubic system $E_4 = 0$ ...(7.12)

[Elements like carbon, silicon and germanium have cubic structures.]

Hence, substituting all the four field values from Equations (7.4), (7.5), (7.11) and (7.12) in Equation (7.1) we get,

$$E_{int} = E + \frac{P}{\varepsilon_o} - \frac{P}{\varepsilon_o} + \frac{P}{3\varepsilon_o} + 0$$

or $$E_{int} = E + \frac{P}{3\varepsilon_o} \quad ...(7.13)$$

The above equation is the Lorentz relation. Thus, it is seen that, the local field is larger than the macroscopic field E by an additional factor $\frac{P}{3\varepsilon_o}$.

7.4 CLAUSIUS-MOSSOTTI RELATION

In physics, the Clausius–Mossotti relation connects the relative permittivity of a dielectric to the polarizability 'α' of the atoms or molecules constituting the dielectric.

Principally, the Clausius–Mossotti relation expresses the dielectric constant, relative permittivity (ε_r), of a material in terms of the atomic polarizibility, α, of the material's constituent atoms and/or molecules, or a homogeneous mixture thereof. It is named after the Italian Physicist Ottaviano–Fabrizio Mossotti and German Physicist Rudolf Clausius. It is equivalent to the Lorentz–Lorenz equation, and is expressed as,

$$\frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{N\alpha}{3\epsilon_0}$$

Where,

- $\varepsilon_r = \varepsilon/\varepsilon_0$ = Dielectric constant of the material.
- ε_0 = Permittivity of free space.
- N = Number density of the molecules (number per cubic meter).
- a = Molecular polarizability in SI units (C•m²/V).

In the case that the material consists of a mixture of two or more species, the right hand side of the above equation would consist of the sum of the molecular polarizability contribution from each species, indexed by ***i*** in the following form:

$$\frac{\epsilon_r - 1}{\epsilon_r + 2} = \sum_i \frac{N_i \alpha_i}{3\epsilon_0}$$

In the CGS system of units the Clausius–Mossotti relation is typically rewritten to show the molecular polarizability volume, $\alpha' = \alpha/(4\pi\varepsilon_0)$ which has units of volume (m^3).

The equation is not based on the dielectric constants but on the indices of refraction. The same formula also defines conductivity and is referred as the Maxwell's formula. When defined for refractivity, then it is termed as the Lorentz–Lorenz equation. It is specifically used when there is no impact from permanent electric dipole moments to the polarization, either because the molecules are nonpolar or because the frequency of the applied field is high.

The Clausius–Mossotti relation can be explained using the polarization density. The polarization density is determined by following three factors:

(1) The electronic polarization α_e produced by opposite displacements of negative electrons and positive nuclei inside the same atoms.

(2) The ionic polarizability α_i produced by opposite displacements of positive and negative ions in the material.

(3) Contributions from the permanent dipole moments of complex ions or molecules at any time when such permanent dipoles are present in the material.

It is expressed in the form,

$$P = N\left(\alpha_e + \alpha_i + \frac{\mu^2}{3kT}\right)$$

The number of atoms or molecules per unit volume is N.

Alternatively, we can state that the Clausius–Mossotti equation for dielectric matter consisting of atoms or non-polar molecules is expressed as,

$$\frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{1}{3\epsilon_0} N\alpha.$$

NOTES

Where ε_0 is the electric constant (permittivity of the vacuum) and N is the number density (number of atoms or molecules per volume).

The index of refraction n of a dielectric is given by,

$$n = \sqrt{\epsilon_r \mu_r} \approx \sqrt{\epsilon_r}.$$

Fundamentally for most dielectric matter the relative magnetic permeability μ_r is very close to unity. Substitution of this value of n gives the Lorentz-Lorenz relation as,

$$\frac{n^2 - 1}{n^2 + 2} = \frac{1}{3\epsilon_0} N\alpha.$$

Derivation

Consider a dielectric with number density N (number of particles per unit volume) in an external electric field **E**. The sum of **E** and an internal field $\mathbf{E}_{int}$ induces a dipole $\mathbf{p}_{ind}$ on each particle. The polarization vector **P** is the sum of the induced dipoles,

$$\mathbf{P} = N\mathbf{p}_{\mathbf{ind}}.$$

From the relation between **P**, the electric displacement **D**, and the electric field **E** follows,

$$\mathbf{P} = \mathbf{D} - \epsilon_0 \mathbf{E} = \epsilon_0(\epsilon_r - 1)\mathbf{E}.$$

To acquire an expression for $\mathbf{p}_{ind}$, consider a single particle (molecule or atom) in a little spherical cavity inside the dielectric. The total field inside this cavity can be approximated by,

$$E_{\mathrm{tot}} = E + E_{\mathrm{int}} = E + \frac{1}{3\epsilon_0} P.$$

Here the absolute magnitudes of the vectors is introduced, which follows because they all lie along the z-axis, the direction of **E**. The field E_{tot} is often referred to as the **Lorentz Local Field**, and in that context designated as E_{loc}. The Lorentz local field approximation is based on the assumption that the long-range interactions are isotropic and so it is only realistic for liquids and isotropic solids.

Subsequently,

$$p_{\mathbf{ind}} = \alpha E_{\mathrm{tot}} = \alpha\left(E + \frac{1}{3\epsilon_0} P\right) = \alpha E\left(1 + \frac{\epsilon_r - 1}{3}\right)$$

Further,

NOTES

$$P = \epsilon_0(\epsilon_r - 1)E = N\alpha E(1 + \frac{1}{3}(\epsilon_r - 1))$$

$$\implies \quad \epsilon_0(\epsilon_r - 1) = \frac{N\alpha}{3}(2 + \epsilon_r).$$

From which the Clausius–Mossotti relation follows directly.

We neglected here the contributions to the total field in the cavity from the other molecules in the cavity. It can be shown that these contributions average out in most dielectrics.

Local Field in Dielectric

Consider that a macroscopic slab of dielectric is placed in an outer electric field **E** in the *z*-direction which polarizes the dielectric, such that a charge density is created on the outer surfaces perpendicular to **E**. Since **E** 'PUSHES' positive charge and 'PULLS' negative charge, hence the sign of the charge density on the outer surfaces appears as shown in the Figure (7.4). The polarization vector **P** points by definition from negative to positive charge. The surface charge densities are in absolute value equal to $|\mathbf{P}| \equiv P$.

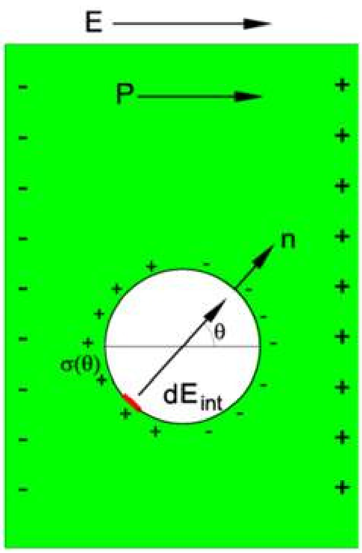


Fig. 7.4** Slab of Dielectric in External Electric Field **E

An infinitesimally small spherical cavity of radius *r* is made in the dielectric and inside this cavity there is vacuum with permittivity electric constant, ε_0. The cavity is so small that the polarization vector **P** is not affected by it. If the cavity had been rectangular with walls parallel to the charged macroscopic surfaces of the slab, the charge density on the walls of the cavity would have been the same (in absolute value) as on the outer surfaces of the slab (*P*), because of electric neutrality. Since the surface of the cavity is spherical, it has the charge density,

NOTES

$$\sigma(\theta) = -\mathbf{n} \cdot \mathbf{P} = -P\cos\theta.$$

Where **n** is a unit length vector perpendicular to the surface of the cavity at the point θ, as shown in the Figure 7.1. By definition, the positive direction of the normal **n** is outward.

An infinitesimal surface element at θ + π,

$$d\Omega = r^2 \,|\sin(\pi+\theta)|\, d\theta d\phi = r^2 \sin\theta \, d\theta d\phi, \quad 0 \le \theta \le \pi.$$

On the wall of the cavity gives a contribution to the internal electric field $d\mathbf{E}_{int}$ parallel to **n**,

$$d\mathbf{E}_{\text{int}} = \mathbf{n}\frac{\sigma(\pi+\theta)d\Omega}{4\pi\epsilon_0 r^2} = -\mathbf{n}\frac{P\cos(\pi+\theta)\; d\Omega}{4\pi\epsilon_0 r^2} = \mathbf{n}\frac{P\cos\theta\sin\theta d\theta d\phi}{4\pi\epsilon_0}.$$

The *z*-component of **n** is cos θ and hence the contribution to the field in the *z* direction is,

$$dE_{\text{int},z} = \frac{P}{4\pi\epsilon_0}(\cos\theta)^2\sin\theta d\theta d\phi.$$

Contributions in other than the *z* direction cancel mutually. Integration over the whole surface gives,

$$E_{\text{int},z} = \iint dE_{\text{int},z} = -\frac{P}{4\pi\epsilon_0}\int_0^{\pi}(\cos\theta)^2 d\cos\theta\int_0^{2\pi}d\phi = \frac{1}{3\epsilon_0}P.$$

The total electric field in the cavity, the 'Lorentz Local Field' is in the *z* direction with the magnitude as,

$$E_{\text{tot}} = E + E_{\text{int}} = E + \frac{1}{3\epsilon_0}P.$$

7.5 POLARIZATION FIELD

1. *Relative Permittivity or Dielectric Constant* ε_r

The dielectric characteristics are determined by the dielectric constant.

The dielectric constant or relative permittivity $\boldsymbol{\varepsilon_r}$ is *defined as, the ratio between the permittivity of the medium* ε *and the permittivity of free space* $\boldsymbol{\varepsilon_o}$.

i.e., $$\boldsymbol{\varepsilon_r} = \frac{\varepsilon}{\varepsilon_o}$$

ε_r is a dimensionless quantity and varies widely from material to material. ε_r has a value of unity for vacuum and for all other dielectrics ε_r is always greater than 1. Since $\varepsilon_r > 1$, we can write $\varepsilon_r = 1 + \chi_e$, where χ_e is called electric susceptibility. Permittivity of a medium (material) indicates, the polarisable nature of a material.

Note:
- ε_r is a constant for a given isotropic material when the applied field is static (dc) and is referred to as static dielectric constant. But, when the material is subjected to an alternating field it becomes a frequency dependent complex quantity.
- ε_r value varies with direction in the case of anisotropic materials.

2. *Polarisation Vector P*

Polarisation vector measures the extent of polarisation in a unit volume of dielectric matter.

Definition - 1 : *It is defined as the induced dipole moment per unit volume of the dielectric.*

P is a vector quantity and, its direction is along the direction of the applied field. If μ is the average induced dipole moment per unit molecule and N is the number of molecules per unit volume then, the polarisation is given by

$$P = N\mu$$

Definition - 2 : *The polarisation P is also defined as the induced surface charge per unit area.*

The above definition is explained below.

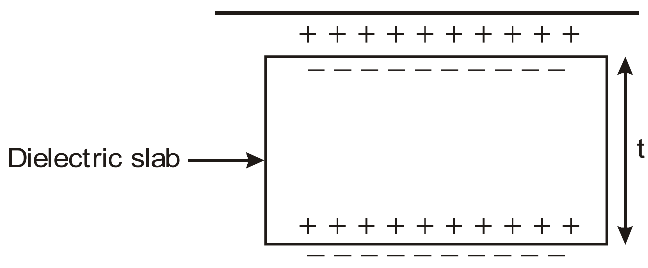


Fig. 7.5 *Dielectric Slab in a Capacitor*

Let, the polarisation of the dielectric slab as a whole give rise to +q and –q induced charges on the respective faces of a dielectric slab of thickness t and volume V kept between the two plates of a capacitor as shown in Figure 7.5. Therefore, the dipole moment of the slab is given by qt. Thus, the dipole moment per unit volume of the dielectric or the polarisation is given by

$$P = \frac{qt}{V}$$

$$P = \frac{qt}{At} \quad [\because V = At, \text{ where A is the area of the slab}]$$

$$\therefore \quad P = \frac{q}{A}$$

Thus, the polarisation is also defined as the induced surface charge per unit area.

NOTES

But, $\frac{q}{A}$ is the induced charge density. Therefore, magnitude of polarisation is equal to the induced charge density.

The unit of polarisation is **Cm^{-2}.**

3. ***Electric Susceptibility*** χ_e

In a large number of dielectrics it is found that the polarisation is directly proportional to the external field (applied) E. For such case,

$$P \propto E$$

Thus, the relation between P and E can be given as,

$$P = \varepsilon_o \chi_e E$$

or

$$\chi_e = \frac{P}{\varepsilon_o E}$$

where χ_e is a constant, called the dielectric susceptibility of the medium.

Definition : *The ratio of polarisation to the net electric field $\varepsilon_o E$ as modified by the induced charges on the surface of the dielectric is called susceptibility.*

4. ***Relation between Polarisation P, Susceptibility*** χ_e ***and the Dielectric Constant*** ε_r

Let us consider a parallel plate capacitor as shown in the Figure 7.6 between which an electric field E_o exists.

If σ is the surface charge density (i.e., charge per unit area) then, from Gauss law,

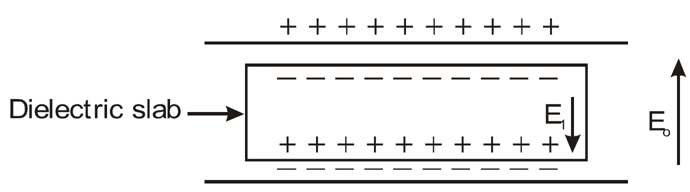


Fig. 7.6 *Fields in a Parallel Plate Capacitor with Dielectric in Between*

$$E_o = \frac{\sigma}{\varepsilon_o} \quad ...(7.14)$$

If a dielectric slab is placed between the plates of the capacitor; then, due to polarisation charges appear on the two faces of the slab and establish another field E_1 within the dielectric. This field will be in a direction opposite to that of E_o.

Therefore, the resultant field E can be given as

$$E = E_o - E_1 \quad ...(7.15)$$

If σ_s is the surface charge density on the slab then, by following equation (7.15), we can write

$$E_1 = \frac{\sigma_s}{\varepsilon_o} \qquad ...(7.16)$$

Therefore, from equations (7.15), (7.16) and (7.17),

$$E = \frac{\sigma}{\varepsilon_o} - \frac{\sigma_s}{\varepsilon_o}$$

or $$\varepsilon_o E = \sigma - \sigma_s \qquad ...(7.17)$$

But, $$\sigma_s = P \quad (\because \text{ Polarisation is Charge/Unit Area}) ...(7.18)$$

Also, by gauss' law, the electric flux density or electric displacement density D is given by

$$D = \sigma \;\; (\text{D is charge/unit area}) \qquad ...(7.19)$$

Therefore, Equation (7.18) can be written as

$$\varepsilon_o E = D - P \qquad ...(7.20)$$

or $$D = \varepsilon_o E + P \qquad ...(7.21)$$

But, from electrostatics we know

$$D = \varepsilon E = \varepsilon_o \varepsilon_r E \qquad ...(7.22)$$

Therefore, Equation (7.19) becomes

$$\varepsilon_o \varepsilon_r E = \varepsilon_o E + P$$

Rearranging the above equation we can write

$$\varepsilon_o E (\varepsilon_r - 1) = P \qquad ...(7.23)$$

or $$\frac{P}{\varepsilon_o E} = (\varepsilon_r - 1) \qquad ...(7.24)$$

But, we know $\frac{P}{\varepsilon_o E} = \chi_e$

$\therefore$ $$\chi_e = \varepsilon_r - 1. \qquad ...(7.25)$$

5. *Polarisability* α

Let us consider an individual atom in a dielectric material. Let, the material be subjected to an electric field E. It is found that, the induced dipolement μ acquired by the atom is proportional to the strength of the electric field E.

i.e., $$\mu \propto E$$

or $$\mu = \alpha E$$

where α is the proportionality constant *called polarisability.* Its unit is $\mathbf{Fm^2}$.

Note: • Polarisability is not a bulk property of the material but, it is the property of an individual atom or molecule.

7.6 LORENTZ FIELD

NOTES

In this equation, the general form of wave equations despite medium properties will be covered. During the process of deriving we will observe the conditions for relations between the scalar electric potential, *'V'* and vector magnetic potential '$\vec{A}$'. This condition is called Lorentz condition. The procedure to obtain the wave equations include, starting from Maxwell's equation and applying the vector identities and simple manipulations of the obtained equations will result in the wave equations.

From Maxwell's second equation,

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{dt}$$

We know that,

$$\vec{B} = \vec{\nabla} \times \vec{A}$$

Therefore,

$$\vec{\nabla} \times \vec{E} = -\frac{\partial}{\partial t}(\vec{\nabla} \times \vec{A})$$

$$\vec{\nabla} \times \vec{E} + \frac{\partial}{\partial t}(\vec{\nabla} \times \vec{A}) = 0$$

$$\vec{\nabla} \times \vec{E} + \vec{\nabla} \times \frac{\partial \vec{A}}{\partial t} = 0$$

$$\vec{\nabla} \times \left[\vec{E} + \frac{\partial \vec{A}}{\partial t}\right] = 0 \qquad (7.26)$$

We know the vector identity that curl of a gradient is zero. Therefore,

$$\vec{\nabla} \times \left(-\vec{\nabla} V\right) = 0 \qquad (7.27)$$

Comparing Equations (7.26) and (7.27), we get,

$$\vec{E} + \frac{\partial \vec{A}}{\partial t} = -\vec{\nabla} V$$

$$\vec{E} = -\vec{\nabla} V - \frac{\partial \vec{A}}{\partial t}$$

$$\vec{E} = -\left[\vec{\nabla} V + \frac{\partial \vec{A}}{\partial t}\right] \qquad (7.28)$$

Taking divergence of Equation (7.28), we get,

NOTES

$$\vec{\nabla}.\vec{E} = \vec{\nabla}.\left[-\left(\vec{\nabla}V + \frac{\partial \vec{A}}{\partial t}\right)\right]$$

$$\vec{\nabla}.\vec{E} = -\left[\nabla^2 V + \frac{\partial}{\partial t}(\vec{\nabla}.\vec{A})\right] \quad (7.29)$$

But from Maxwell's first equation,

$$\vec{\nabla}.\vec{E} = \frac{\rho_V}{\epsilon}$$

Therefore, equating the above equation with Equation (7.30),

$$\frac{\rho_V}{\epsilon} = -\left[\nabla^2 V + \frac{\partial}{\partial t}(\vec{\nabla}.\vec{A})\right]$$

Or

$$\nabla^2 V + \frac{\partial}{\partial t}(\vec{\nabla}.\vec{A}) = -\frac{\rho_V}{\epsilon} \quad (7.30)$$

So far, we have used Maxwell's equation for electric field and now let us use Maxwell's equation for magnetic field to couple the two fields to arrive at the electromagnetic waves. Considering, Maxwell's fourth equation,

$$\vec{\nabla} \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{dt}$$

But, $\vec{B} = \mu\vec{H}$. Therefore,

$$\vec{\nabla} \times \frac{\vec{B}}{\mu} = \vec{J} + \frac{\partial \vec{D}}{dt}$$

$$\vec{\nabla} \times \vec{B} = \mu\vec{J} + \mu\frac{\partial \vec{D}}{dt}$$

Also, $\vec{D} = \epsilon\vec{E}$

$$\vec{\nabla} \times \vec{B} = \mu\vec{J} + \mu\epsilon\frac{\partial \vec{E}}{dt} \quad (7.31)$$

Substituting for $\vec{E}$, from Equation (7.31) , we get,

$$\vec{\nabla} \times \vec{B} = \mu\vec{J} + \mu\epsilon\frac{\partial}{dt}\left[-\vec{\nabla}V - \frac{\partial \vec{A}}{\partial t}\right]$$

$$\vec{\nabla} \times \vec{B} = \mu\vec{J} - \mu\epsilon\vec{\nabla}\frac{\partial V}{dt} - \mu\epsilon\frac{\partial^2 \vec{A}}{\partial t^2}$$

NOTES

But $\vec{B} = \vec{\nabla} \times \vec{A}$, Hence,

$$\vec{\nabla} \times \vec{\nabla} \times \vec{A} = \mu\vec{J} - \mu\epsilon\vec{\nabla}\frac{\partial V}{dt} - \mu\epsilon\frac{\partial^2 \vec{A}}{\partial t^2} \tag{7.32}$$

Applying vector identity to the LHS of Equation (7.32), we get,

$$\vec{\nabla} \times \vec{\nabla} \times \vec{A} = \vec{\nabla}(\vec{\nabla}.\vec{A}) - \nabla^2\vec{A}$$

$$\vec{\nabla}(\vec{\nabla}.\vec{A}) - \nabla^2\vec{A} = \mu\vec{J} - \mu\epsilon\vec{\nabla}\frac{\partial V}{dt} - \mu\epsilon\frac{\partial^2 \vec{A}}{\partial t^2} \tag{7.33}$$

Observing Equation (7.33), we find that scalar potential V and vector potential $\vec{A}$ can be separated and decoupled. Therefore for vector potential, $\vec{A}$, Equation (7.32) becomes,

$$-\nabla^2\vec{A} = \mu\vec{J} - \mu\epsilon\frac{\partial^2 \vec{A}}{\partial t^2}$$

Or

$$\nabla^2\vec{A} - \mu\epsilon\frac{\partial^2 \vec{A}}{\partial t^2} = \mu\vec{J} \tag{7.34}$$

Similarly, it is good to separate for scalar potential V in terms of $\vec{A}$ because we obtain a relation relating $\vec{A}$ and V known as ***Lorentz condition*** for potentials.

$$\vec{\nabla}(\vec{\nabla}.\vec{A}) = -\mu\epsilon\vec{\nabla}\frac{\partial V}{dt}$$

$$= \vec{\nabla}\left(-\mu\epsilon\frac{\partial V}{dt}\right)$$

$$\vec{\nabla}.\vec{A} = -\mu\epsilon\frac{\partial V}{dt} \tag{7.35}$$

The above relation is known as **Lorentz condition for potentials**.

Recalling Equation (7.35),

$$\nabla^2 V + \frac{\partial}{\partial t}(\vec{\nabla}.\vec{A}) = -\frac{\rho_V}{\epsilon}$$

Substituting for $\vec{\nabla}.\vec{A}$ from Equation (7.34) in Equation (7.35) above,

$$\nabla^2 V + \frac{\partial}{\partial t}\left(-\mu\epsilon\frac{\partial V}{dt}\right) = -\frac{\rho_V}{\epsilon}$$

$$\nabla^2 V - \mu\epsilon \frac{\partial^2 V}{dt^2} = -\frac{\rho_V}{\epsilon} \tag{7.36}$$

Recalling Equation (7.36) as below,

NOTES

$$\nabla^2 \vec{A} - \mu\epsilon \frac{\partial^2 \vec{A}}{\partial t^2} = \mu\vec{J}$$

The above two equations are called as ***wave equations***. Equations (7.35) and (7.36) are decoupled equations of $\vec{A}$ and V, whereas Equations (7.34) and (7.35) are coupled equations, in which and are interlinked.

Free Space Wave Equations

In free space, $\rho_V = 0$ and $\vec{J} = 0$ and hence, the wave equations simplify to,

$$\nabla^2 V - \mu\epsilon \frac{\partial^2 V}{dt^2} = -\frac{\rho_V}{\epsilon} \tag{7.37(a)}$$

And

$$\nabla^2 \vec{A} - \mu\epsilon \frac{\partial^2 \vec{A}}{\partial t^2} = \mu\vec{J} \tag{7.37(b)}$$

From electrostatics and magnetostatics,

$$V = -\oint_L \vec{E}.\vec{dl}$$

And

$$\vec{\nabla} \times \mu\vec{H} = \vec{A}$$

Eqnation (7.37) can be rewritten as,

$$\nabla^2 \vec{E} - \mu\epsilon \frac{\partial^2 \vec{E}}{dt^2} = 0 \tag{7.37(b)}$$

And

$$\nabla^2 \vec{A} - \mu\epsilon \frac{\partial^2 \vec{A}}{\partial t^2} = \mu\vec{J} \tag{7.37(b)}$$

Uniform Plane Waves

Plane waves are waves with same phase at all points of existence. Uniform plane waves are plane waves with constant amplitude.

Consider an electric field wave equation from Equation (7.37(a))

NOTES

$$\nabla^2\vec{E} - \mu\epsilon\frac{\partial^2\vec{E}}{dt^2} = 0$$

$$\nabla^2\vec{E} = \mu\epsilon\frac{\partial^2\vec{E}}{dt^2}$$

We know that, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ and

$\vec{E} = E_x\overrightarrow{a_x} + E_y\overrightarrow{a_y} + E_z\overrightarrow{a_z}$. Therefore,

$$\frac{\partial^2 E_x}{\partial x^2}\overrightarrow{a_x} + \frac{\partial^2 E_y}{\partial y^2}\overrightarrow{a_y} + \frac{\partial^2 E_z}{\partial z^2}\overrightarrow{a_z} = \mu\epsilon\left[\frac{\partial^2 E_x}{\partial t^2}\overrightarrow{a_x} + \frac{\partial^2 E_y}{\partial t^2}\overrightarrow{a_y} + \frac{\partial^2 E_z}{\partial t^2}\overrightarrow{a_z}\right]$$

In the above equation, it should be noted that $\frac{\partial^2 E_y}{\partial y^2} = 0$ and likewise for unequal variables. Splitting the above three dimensional vector equation to a one-dimensional scalar equation,

$$\frac{\partial^2 E_x}{\partial x^2} = \mu\epsilon\frac{\partial^2 E_x}{\partial t^2} \quad (7.38(a))$$

$$\frac{\partial^2 E_y}{\partial y^2} = \mu\epsilon\frac{\partial^2 E_y}{\partial t^2} \quad (7.38(b))$$

$$\frac{\partial^2 E_z}{\partial z^2} = \mu\epsilon\frac{\partial^2 E_z}{\partial t^2} \quad (7.38(c))$$

Also, in free space, where the electromagnetic waves travel, (they can also travel through different medium), $\rho_V = 0$ and $\vec{J} = 0$. Therefore, from Maxwell's first equation,

$$\vec{\nabla}.\vec{D} = 0$$

$$\vec{\nabla}.\epsilon\vec{E} = 0$$

$$\vec{\nabla}.\vec{E} = 0$$

$$\Rightarrow \left(\frac{\partial}{\partial x}\overrightarrow{a_x} + \frac{\partial}{\partial y}\overrightarrow{a_y} + \frac{\partial}{\partial z}\overrightarrow{a_z}\right).\left(E_x\overrightarrow{a_x} + E_y\overrightarrow{a_y} + E_z\overrightarrow{a_z}\right) = 0$$

$$\frac{\partial}{\partial x}E_x + \frac{\partial}{\partial y}E_y + \frac{\partial}{\partial z}E_z = 0$$

Since, E_x is travelling in the x –direction, $\frac{\partial E_y}{\partial y} = \frac{\partial E_z}{\partial z} = 0$. Then, $\frac{\partial E_x}{\partial x}$ represents that no variation of E_x in x-direction and also $\vec{E}$ is independent of y and z. Differentiating with respect to x,

$$\frac{\partial^2 E_x}{\partial x^2} = 0$$

The solution of the above second order differential equation exists only if,

$$E_x = 0 \quad or \quad E_x = K(constant)$$

If $E_x = K$, then E_x is not a wave, but a constant dc line. Hence, a uniform plane wave travelling in x –direction do not have an component of $\vec{E}$. Similarly for the other two directions y and z.

For the magnetic field vector, following the similar approach, from Maxwell's third equation,

$$\vec{\nabla}.\vec{B} = 0$$

$$\vec{\nabla}.\mu\vec{H} = 0$$

$$\vec{\nabla}.\vec{H} = 0$$

$$\Rightarrow \left(\frac{\partial}{\partial x}\overrightarrow{a_x} + \frac{\partial}{\partial y}\overrightarrow{a_y} + \frac{\partial}{\partial z}\overrightarrow{a_z}\right).\left(H_x\overrightarrow{a_x} + H_y\overrightarrow{a_y} + H_z\overrightarrow{a_z}\right) = 0$$

$$\frac{\partial}{\partial x}H_x + \frac{\partial}{\partial y}H_y + \frac{\partial}{\partial z}H_z = 0$$

Since, H_x is travelling in the x –direction, $\frac{\partial H_y}{\partial y} = \frac{\partial H_z}{\partial z} = 0$. $\vec{H}$ is independent of y and z. Therefore,

$$\frac{\partial H_x}{\partial x} = 0 \Rightarrow \frac{\partial^2 H_x}{\partial x^2} = 0$$

Since H_x cannot be constant, to satisfy the above second order differential equation, $H_x = 0$ for uniform plane wave.

Properties of Electromagnetic Waves

Electromagnetic waves transport energy or information from one point to the other. Few examples of electromagnetic waves include the waves in the electromagnetic spectrum as shown in Figure (7.7). Few electromagnetic waves include X-rays, Gamma rays, microwave, TV signals, radar signals, light rays, etc. The electromagnetic waves are also called as Hertzian waves.

NOTES

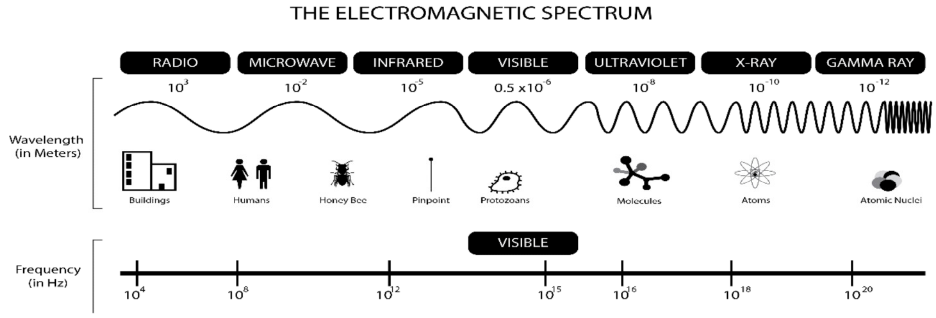


Fig. 7.7 *Electromagnetic Spectrum*

Characteristics of EM Waves

Following are the characteristics of EM waves.

1. They travel at a speed of light in vacuum.
2. They travel similar to the waves with the same their same property.
3. They radiate away from the source
4. They can travel across any medium
5. EM waves are generated by vibration of electrons resulting in energy emission called as electromagnetic radiation.
6. Electromagnetic waves have both electric and magnetic components.
7. Electric and magnetic components are orthogonal (perpendicular) to each other.
8. The direction of wave propagation will be orthogonal to the electric and magnetic waves. Such waves are called Transverse ElectroMagnetic waves (TEM waves).

Parameters of Wave

A simple wave is a sinusoidal signal as represented as in Figure (7.8).

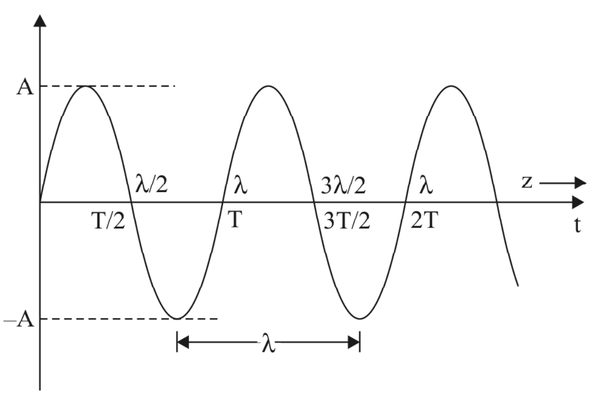


Fig. 7.8 *EM Wave*

NOTES

Let $\lambda = wavelength\ (m)$

$T = Time\ period\ (S)$

$u = speed\ (m/s)$

$\therefore \qquad u = \frac{\lambda}{T} = f\lambda \qquad [f = 1/T]$

Let $\omega = angular\ frequency\ (rad/s)$

$\beta = phase\ constant\ or\ wave\ number\ (rad/m)$

$\omega = 2\pi f\ (rad/s)$

$$\beta = \frac{\omega}{u} = \frac{2\pi f}{u}$$

$$\beta = \frac{2\pi f}{f\lambda}$$

$$\beta = \frac{2\pi}{\lambda}$$

Check Your Progress

1. Define the term polarisation.
2. What do you mean by the local electric field?
3. Elucidate on the Clausius–Mossotti relation.
4. State the relative permittivity or dielectric constant r.
5. Elaborate on the polarisation vector P.
6. Interpret the electric susceptibility.
7. Define the uniform plane waves.
8. Explain the characteristics of EM waves.

7.7 ANSWERS TO CHECK YOUR PROGRESS QUESTIONS

1. Polarisation is defined as the process of creating or inducing dipoles in a dielectric material by an external electric field. The polarisation increases with the field up to the critical value.
2. The electric field acting at an atom in a dielectric known as the internal field or local field E_{int} is different from the applied external field. The internal field, or the local field, is the electric field acting at an atom of a solid or liquid dielectric subjected to an external field.

NOTES

3. In condensed matter physics, the Clausius–Mossotti's relation connects the relative permittivity of a dielectric to the polarizability 'α' of the atoms or molecules constituting the dielectric.
4. The dielectric characteristics are determined by the dielectric constant. The dielectric constant or relative permittivity ε_r is defined as, the ratio between the permittivity of the medium ε and the permittivity of free space ε_o.
5. Polarisation vector measures the extent of polarisation in a unit volume of dielectric matter. It is defined as the induced dipole moment per unit volume of the dielectric. The polarisation P is also defined as the induced surface charge per unit area.
6. The ratio of polarisation to the net electric field $\varepsilon_o E$ as modified by the induced charges on the surface of the dielectric is called susceptibility.
7. Plane waves are waves with same phase at all points of existence. Uniform plane waves are plane waves with constant amplitude.
8. Following are the characteristics of EM waves:
   - o They travel at a speed of light in vacuum.
   - o They travel similar to the waves with the same their same property.
   - o They can travel across any medium
   - o Electromagnetic waves have both electric and magnetic components
   - o They radiate away from the source
   - o EM waves are generated by vibration of electrons resulting in energy emission called as electromagnetic radiation.

7.8 SUMMARY

- Polarisation is defined as the process of creating or inducing dipoles in a dielectric material by an external electric field. The polarisation increases with the field up to the critical value.
- The electric field acting at an atom in a dielectric known as the internal field or local field E_{int} is different from the applied external field. The internal field, or the local field, is the electric field acting at an atom of a solid or liquid dielectric subjected to an external field.
- In condensed matter physics, the Clausius–Mossotti's relation connects the relative permittivity of a dielectric to the polarizability 'α' of the atoms or molecules constituting the dielectric.
- The dielectric characteristics are determined by the dielectric constant. The dielectric constant or relative permittivity is defined as, the ratio between the permittivity of the medium and the permittivity of free space .

- Polarisation vector measures the extent of polarisation in a unit volume of dielectric matter. It is defined as the induced dipole moment per unit volume of the dielectric. The polarisation *P* is also defined as the induced surface charge per unit area.
- The ratio of polarisation to the net electric field as modified by the induced charges on the surface of the dielectric is called susceptibility.
- Plane waves are waves with same phase at all points of existence. Uniform plane waves are plane waves with constant amplitude.
- Electromagnetic waves have both electric and magnetic components. EM waves are generated by vibration of electrons resulting in energy emission called as electromagnetic radiation.

7.9 KEY WORDS

- **Polarisation:** Polarisation is defined as the process of creating or inducing dipoles in a dielectric material by an external electric field. The polarisation increases with the field up to the critical value.
- **Clausius–Mossotti's relation:** The Clausius–Mossotti's relation connects the relative permittivity of a dielectric to the polarizability 'α' of the atoms or molecules constituting the dielectric.
- **Dielectric constant:** The dielectric constant or relative permittivity is defined as, the ratio between the permittivity of the medium and the permittivity of free space .
- **Polarisation vector:** It is defined as the induced dipole moment per unit volume of the dielectric. The polarisation *P* is also defined as the induced surface charge per unit area.
- **Susceptibility:** The ratio of polarisation to the net electric field as modified by the induced charges on the surface of the dielectric is called susceptibility.
- **Uniform plane waves:** Uniform plane waves are plane waves with constant amplitude.

7.10 SELF ASSESSMENT QUESTIONS AND EXERCISES

Short-Answer Questions

1. What is polarisation?
2. Define the term local electric field.
3. Interpret the Clausius–Mossotti relation.

NOTES

4. State the relative permittivity or dielectric constant r.
5. Illustrate the polarisation vector P.
6. Elaborate on the electric susceptibility.
7. What do you mean by the uniform plane waves?
8. Define the characteristics of EM waves.

Long-Answer Questions

1. Discuss briefly the concept of polarisation giving appropriate examples.
2. Explain the local electric field.
3. Analyse the Clausius–Mossotti's relation.
4. Describe the polarization field with the help of examples.
5. Elaborate on the Lorentz field.

7.11 FURTHER READINGS

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UNIT 8 DIELECTRIC CONSTANT AND POLARIZABILITY

Structure

8.0 Introduction
8.1 Objectives
8.2 Dielectric Constant
8.3 Polarizability: Electronic, Ionic-Poezo
8.4 Pyro and Ferro Electric Properties of Crystals
8.5 Answers to Check Your Progress Questions
8.6 Summary
8.7 Key Words
8.8 Self Assessment Questions and Exercises
8.9 Further Readings

8.0 INTRODUCTION

Dielectric constant or relative permittivity, of a material is its (absolute) permittivity expressed as a ratio relative to the vacuum permittivity. Permittivity is a materials property that affects the Coulomb force between two point charges in the material. Relative permittivity is the factor by which the electric field between the charges is decreased relative to vacuum.

Similarly, relative permittivity is the ratio of the capacitance of a capacitor using that material as a dielectric, compared with a similar capacitor that has vacuum as its dielectric. Relative permittivity is also commonly known as the dielectric constant, a term still used but deprecated by standards organizations in engineering as well as in chemistry.

The historical term for the relative permittivity is dielectric constant. It is still commonly used, but has been deprecated by standards organizations, because of its ambiguity, as some older authors used it for the absolute permittivity å. The permittivity may be quoted either as a static property or as a frequency-dependent variant. It has also been used to refer to only the real component $å'_r$ of the complex-valued relative permittivity.

NOTES

The polarizability of an atom or molecule is defined as the ratio of its induced dipole moment to the local electric field; in a crystalline solid, one considers the dipole moment per unit cell. Note that the local electric field seen by a molecule is generally different from the macroscopic electric field that would be measured externally. This discrepancy is taken into account by the Clausius–Mossotti relation, which connects the bulk behaviour (polarization density due to an external electric field according to the electric susceptibility $\chi = \varepsilon_r - 1)$ with the molecular polarizability α due to the local field.

Polarizability usually refers to the tendency of matter, when subjected to an electric field, to acquire an electric dipole moment in proportion to that applied field. It is a property of all matter, inasmuch as matter is made up of elementary particles which have an electric charge, namely protons and electrons. When subject to an electric field, the negatively charged electrons and positively charged atomic nuclei are subject to opposite forces and undergo charge separation. Polarizability is responsible for a material's dielectric constant and, at high (optical) frequencies, its refractive index.

In this unit, you will study about the dielectric constant, polarizability: electronic, ionic– piezo – pyro and ferro electric properties of crystals.

8.1 OBJECTIVES

After going through this unit, you will be able to:

- Understand the dielectric constant
- Elucidate on the polarizability: electronic, ionic–piezo
- Analyse the pyro and ferro electric properties of crystals

8.2 DIELECTRIC CONSTANT

Dielectric loss is a major problem involving heat generation and is dominating in high voltage application.

When an ac voltage is applied to a pure dielectric material like vacuum or purified gases, there is no consumption of energy. As a result, the charging current leads the applied voltage by an angle 90° as shown in Figure 8.1(*a*) and the polarisation of the dielectric is in phase with the voltage.

But, when an ac voltage is applied to commercial dielectrics, the charging current does not lead the applied voltage by exactly 90°; but, is always less than 90° as shown in Figure 8.1(*b*).

The complementary angle $\delta = 90 - \theta$ is called the dielectric loss angle. This angle is a measure of the power or heat dissipated in each cycle. In most of the dielectrics this angle δ is negligible.

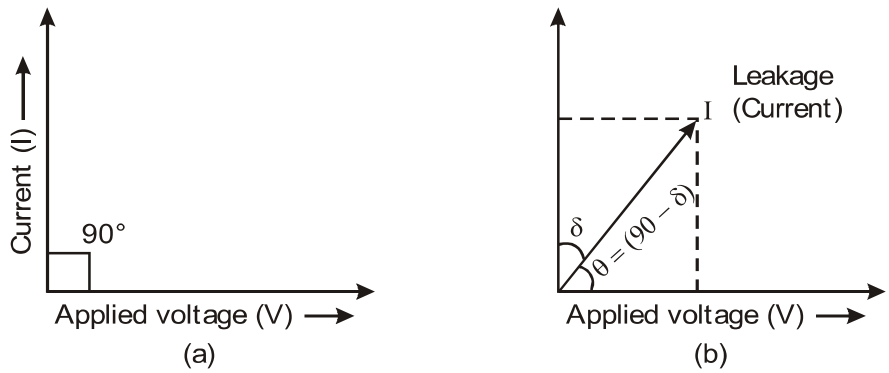


Fig. 8.1 *Dielectric Loss*

The dielectric power loss for a dielectric material used in a capacitor with capacitance C and applied voltage V is given by

$$P = VI\cos\theta$$

where V is the applied voltage in volts

I is the current through the capacitor in amp.

The value of I is given by the relation

$$I = \frac{V}{X_C}$$, where, X_C is the capacitive reactance

given by $$X_C = \frac{1}{2\pi fC}$$

$$\therefore \quad P = V\frac{V}{X_C}\cos(90° - \delta) \qquad [\because \theta = 90° - \delta]$$

$$= V^2 \; 2\pi f C \; \sin\delta \qquad [\because \cos(90° - \delta) = \sin\delta]$$

But, since δ is negligibly small in most of the dielectrics

$$\sin\delta = \tan\delta$$

$$\therefore \quad P = 2\pi V^2 f C \; \tan\delta$$

Here, tanδ is called the power factor. It is also referred to as tangent loss. When the factors like voltage, frequency and capacitance are constant, the dielectric loss is dependent only on δ. The dielectric loss should be low in a dielectric material.

Factors Affecting Dielectric Loss

The dielectric loss increases with:

1. High frequency of the applied voltage.
2. High applied voltage.
3. High temperature and humidity.

NOTES

Dielectric breakdown

Whenever the voltage applied to a dielectric material exceeds a critical value, a large amount of current flows through it. As a result of this, the dielectric loses its insulating property. This phenomena is known as dielectric breakdown.

Thus, breakdown indicates the failure of the dielectric material.

The electric field at which this breakdown occurs is called the dielectric strength. Also,

$$\text{Dielectric strength} = \frac{\text{Breakdown voltage}}{\text{Thickness of the dielectric}}$$

It is expressed in kV/cm. Dielectric strength decreases with increase of temperature and humidity.

Important types of dielectric breakdown and their mechanism by which, the breakdown takes place are briefly explained below.

Important types of breakdown

1. Intrinsic breakdown.
2. Thermal breakdown.
3. Electrochemical breakdown.
4. Discharge breakdown.
5. Defect breakdown.

1. Intrinsic Breakdown

When the electric field applied to a dielectric material exceeds a critical value, there is an electric breakdown due to physical deterioration of the dielectric material. When the applied field is large, some of the electrons from the valence band cross over the conduction band giving rise to large conduction current. As a result of this, a large current flows through the dielectric and the subsequent breakdown is called as an intrinsic breakdown or zener breakdown.

Note: • The liberation of electrons from the valence band due to large charge displacement by the higher electric field is called internal field emission of electrons.

The liberated electrons moving under high accelerating electric force collide with atoms or molecules of the dielectric and release more electrons by continuous breaking of covalent bonds. As a result of this, a large current flows through the dielectric and the subsequent breakdown is called as *avalanche breakdown.*

Characteristics or Properties

1. This can occur at any temperature.
2. This requires large electric field to occur.

3. Mostly this kind of breakdown occurs in thin samples only.
4. This does not depend on the electrode configuration and the shape of the material.

NOTES

2. Thermal Breakdown

When there is excessive increase in the temperature of the dielectric a local melting occurs due to less heat dissipation than heat generated. Hence, mobility of charge carriers is increased, and enormous current flows through the material thus, leading to thermal breakdown.

Characteristics or Properties

1. This can occur only at high temperatures.
2. The breakdown time is of the order of few milli seconds.
3. Mostly this occur in lossy dielectrics.
4. The strength of the electric field to create dielectric breakdown depends upon the material size and shape.
5. Since dielectric loss is directly proportional to frequency, the electric field to create dielectric breakdown will be smaller for alternating fields and higher for (static) dc fields.

3. Electrochemical Breakdown

Dielectric breakdown due to the formation of electro chemical reaction or chemical reaction in a dielectric material is called electrochemical breakdown. This electrochemical breakdown is closely related to the thermal breakdown. An increase of temperature results in an increase of mobility of ions and also an increase in leakage current. Hence, electrochemical reaction takes place and thus, leading to dielectric breakdown.

A chemical reaction within the dielectric material can occur not only by the application of the electric field but also can occur by so many ways.

Characteristics or Properties

1. This type of breakdown is accelerated by atmospheric air. For example, rubber gets converted to rubber oxide in the ozone atmosphere with the formation of cracks on it. Since it is converted into oxide, its dielectric properties get degraded.
2. To avoid this type of breakdown foreign materials should not be mixed with pure insulating materials.
3. This type of breakdown is highly favoured at high temperatures; at which, the stability of chemical properties decreases.
4. This breakdown is very common in dielectric materials with permanent dipoles. The dipoles produce a large leakage current, and subsequently leading to this breakdown.
5. Electrochemical breakdown is accelerated by humidity.

4. Discharge Breakdown

Discharge breakdown occurs due gaseous discharge taking place in occluded gas bubbles. Since, the ionisation potential of gaseous atoms are smaller than the solid atoms of the dielectric material, the gaseous atoms ionise first and bombard the solid atoms of the dielectric causing electrical deterioration resulting in breakdown.

Characteristics or Properties

1. This type of breakdown is highly favoured where there are a large number of occluded gas bubbles.
2. This can occur even at low voltages.

5. Defect Breakdown

The presence of cracks or pores at the surface of the material leads to defect breakdown due to the collection of moisture and other impurities at these defect sites.

Characteristics or Properties

The life of the insulation of the dielectric material depends upon, the number of discharges taking place inside the material.

Properties of a good dielectric material

To avoid breakdown, the dielectric material should possess the following properties.

1. It should have high resistivity to reduce leakage current. (like sulphur).
2. It should have high dielectric strength. (like mica).
3. It should have high mechanical strength. (like steel).
4. It should have high fire resistance. (like silica).
5. It should have high chemical inertness. (like platinum) [i.e., it should be resistant to oils, liquids, gas, acids and alkalies].
6. It should have low thermal expansion. (like invar).
7. It should have high thermal conductivity. (like silver).
8. It should have low dielectric loss. (like vacuum).
9. It should have low water absorption quality. (like paraffin wax).
10. It should have high quality surface finish. (like ebonite).

Types of Dielectric Materials

Dielectric materials can be solids, liquids or gases. A high vacuum can also be used as a dielectric eventhough its relative dielectric constant is only unity.

Solid dielectrics are most commonly used in electrical engineering and are very good insulators.

NOTES

Examples: Porcelain, glass, plastics, rubber, cotton, wood, mica etc.

Liquid dielectric materials are basically of three different types, which include (i) Mineral insulating oils, (ii) Synthetic insulating oils and (iii) Miscellaneous insulating oils.

The function of insulating liquids is to provide electrical insulation and to dissipate heat (cooling agent).

Examples: Transformer oil, cable oil, capacitor oil, vegetable oil, vaseline, silicon liquids. sovol, soutol, etc.

Gaseous dielectric material are used both as an insulator and as a cooling agent.

Examples: Air, hydrogen, nitrogen, helium, sulphurdioxide, propane, methane, sulphur hexafloride, ethane, etc.

Specific Applications of Dielectrics

The dielectric materials based on their nature of state has a variety of applications in electrical engineering field.

The applications of different dielectric materials in capacitors and transformers with their functions are listed below.

Capacitors

The major role of dielectric materials in capacitor is to store electrical energy. Based on the nature of the dielectric material used, the capacitors fall into different groups.

1. Capacitors with vacuum, air or other gases as dielectric are used in radio frequency and low frequency measuring circuits.
2. Capacitors with mineral oil as dielectric are used in high voltage applications, where a large value of capacitance is required.
3. Capacitors with a combination of solid and liquid dielectrics are used in the applications where precision is not so important but a high value capacitance is required.

   In electric power distribution system for power factor correction, these type of capacitors are used. ***Examples:*** Glass, mica, oil impregnated paper dielectric, mineral oil, castor oil etc.
4. Capacitors with only solid dielectrics like sodium, glass, titanium oxide etc, are used in laboratory as standard capacitor.

Transformer

In transformers the dielectrics are used as an insulator as well as a cooling agent.

The applications of different types of solid, liquid and gaseous dielectric material with their function in transformer are listed below.

1. Solid Dielectric Materials

1. Fibrous (class A) materials are used in air cooled and oil cooled transformers.
2. Cotton tape is used for insulating the conductors of oil cooled transformer.
3. High quality synthetic resin bonded paper in the form of cylinders is used as an insulator between core and coils and also between primary and secondary windings.
4. Press board or press paper is used as a filling, and as a packing material between coil.

2. Liquid Dielectric Materials

1. *Transformer oil* - It is a class of mineral insulating oil and is used as a coolant. It also maintains the insulation of the winding.
2. Fluorocarbon liquids are used in large transformers to give high heat transfer rates together with high dielectric strength.

3. Gaseous Dielectric Materials

(*i*) The usage of nitrogen in transformer prevents oxidation and reduces the rate of deterioration.

(*ii*) Sulphur hexafloride dielectric, is an electronegative gas used in transformers. It is non- toxic, non-inflammable and chemically inert.

8.3 POLARIZABILITY: ELECTRONIC, IONIC-POEZO

There are four different types of mechanisms through which electrical polarisation can occur in a dielectric material when they are subjected to an external electric field.

They are:

1. Electronic polarisation.
2. Ionic polarisation.
3. Orientation polarisation.
4. Space charge or Interfacial polarisation.

1. Electronic Polarisation

The electronic polarisation occurs, due to the displacement of the positively charged nucleus and the negatively charged electron cloud in opposite directions within a dielectric material upon applying an external electric field E.

Thus, the separation created between the charges induces a dipole. This process occurs throughout the material and the material as a whole will be polarised. Electronic polarisation is more in liquid and solid dielectrics than in gases.

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Therefore, the induced dipole moment = $\mu = \alpha_e E$
where α_e is electronic polarisability.

The electronic polarisability for a rare gas atom is given by

$$\alpha_e = \frac{\varepsilon_o(\varepsilon_r - 1)}{N}$$ where N is the number of atoms per unit volume.

Expression for Electronic Polarisability α_e

Let us consider one of the constituent atom of a dielectric material in the absence of an electric field E. Let the radius of the atom be R and its atomic number be Z as shown in Figure 8.2. Here, the nucleus of charge Ze is surrounded by an electronic cloud of charge –Ze. In the atom, the negative charge distribution due to its electron is spherically symmetric.

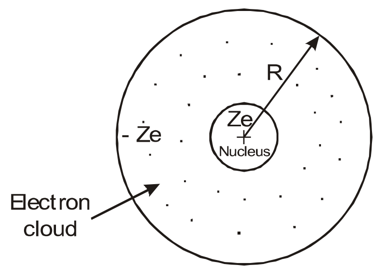


***Fig. 8.2** Atom of a Dielectric Material in the Absence of Electric Field*

Therefore, the charge density for electron cloud is given by

$$\rho = \frac{-Ze}{\frac{4}{3}\pi R^3} = \frac{-3}{4}\left(\frac{Ze}{\pi R^3}\right) \qquad ...(8.1)$$

But, when an electric field is applied, the nucleus and the electron cloud experience a Lorentz force of magnitude ZeE in opposite directions. Hence, the nucleus and the electron cloud are pulled by a distance.

Since, the nucleus is much heavier than the electron cloud it is assumed that only the electron cloud is displaced upon applying an electric field. Let the electron cloud displacement be *x* with respect to the centre of the nucleus.

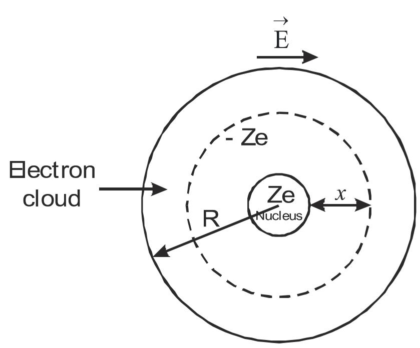


***Fig. 8.3** Atom of a Dielectric Material in the Presence of Electric Field*

NOTES

Hence, the Lorentz force acting over the electron cloud is – ZeE ...(8.2)

But, according to Gauss theorem a coulomb attractive force is said to act over the nucleus due to the electron cloud in a sphere of radius x and this force tends to oppose the displacement.

Thus, the Coulomb force = Ze × E ...(8.3)

Based on Coulomb's theorem

$$E = \frac{\text{Total charge enclosed in a sphere of radius } x\ (q)}{4\pi\varepsilon_o x^2} \quad ...(8.4)$$

Note: • **Coulomb's Theorem Statement:** The electric field at any point in a charged conductor is $1/\varepsilon_o$ times the surface charge density, i.e., charge per unit area.

But, the total charge enclosed in a sphere of radius x is $q = \rho \times \frac{4}{3}\pi x^3$ ...(8.5)

where ρ is negative charge density and $\frac{4}{3}\pi x^3$ is volume of the sphere of radius x.

Substituting for ρ from equation (1) we get,

$$q = \frac{-3}{4}\left(\frac{Ze}{\pi R^3}\right) \times \frac{4}{3}\pi x^3$$

or
$$q = \frac{-Zex^3}{R^3} \quad ...(8.6)$$

Substituting for q in equation (8.6) we get, $E = \frac{-Zex^3}{R^3} \times \frac{1}{4\pi\varepsilon_o x^2}$ ...(8.7)

Hence, equation (8.5) can be given as (substituting for E from equation (7))

$$\text{Coulomb force} = Ze \times \frac{-Zex^3}{R^3} \times \frac{1}{4\pi\varepsilon_o x^2} = \frac{-Z^2e^2x}{4\pi\varepsilon_o R^3} \quad ...(8.8)$$

These two forces, i.e., the Lorentz force and the coulomb force are equal in magnitude but opposite in direction. As a result, a equilibrium is reached. Hence, at equilibrium

$$\text{Lorentz force} = \text{Coulomb force}$$

$$-ZeE = \frac{-Z^2e^2x}{4\pi\varepsilon_o R^3} \quad ...(8.9)$$

or
$$E = \frac{Zex}{4\pi\varepsilon_o R^3} \quad ...(8.10)$$

Hence,
$$x = \frac{4\pi\varepsilon_o R^3}{Ze} E \quad ...(8.11)$$

NOTES

Thus, the displacement of the electron cloud is proportional to the applied field E. Due to this displacement the atom acts as a dipole.

Therefore, the induced dipolement

$$\mu = Ze \times x$$

$$= (Ze)\left(\frac{4\pi\varepsilon_o R^3}{Ze} E\right) \quad \text{(Substituting for } x \text{ from}$$

equation (9))

or $\mu = 4\pi\varepsilon_o R^3 E$ ...(8.12)

But, $\mu = \alpha_e E$ ...(8.13)

Comparing equation (8.12) and (8.13), we have

$$\alpha_e = 4\pi\varepsilon_o R^3 \qquad ...(8.14)$$

Thus, the electronic polarisability is proportional to the volume of the atom and is independent of temperature.

The polarisation vector P = Nμ

$\therefore$ $P = N\,\alpha_e\,E$ ...(8.15)

But, we know that $P = \varepsilon_o E\,(\varepsilon_r - 1)$ ...(8.16)

$\therefore$ Equating equations (8.15) and (8.16), we get

$$N\,\alpha_e\,E = \varepsilon_o E\,(\varepsilon_r - 1)$$

or $\alpha_e = \dfrac{\varepsilon_o(\varepsilon_r - 1)}{N}$ ...(8.17)

2. Ionic Polarisation

Ionic polarisation occur only in ionic solids such as NaCl which possess ionic bonds. It does not occur in covalent crystals such as diamond, silicon and germanium.

When ionic solids are subjected to an external electric field, the adjacent ions of opposite sign undergo displacement as shown in Figure 8.6. The displacement may cause either an increase or decrease in the distance of separation between the atoms depending upon the location of the ion pair in the lattice.

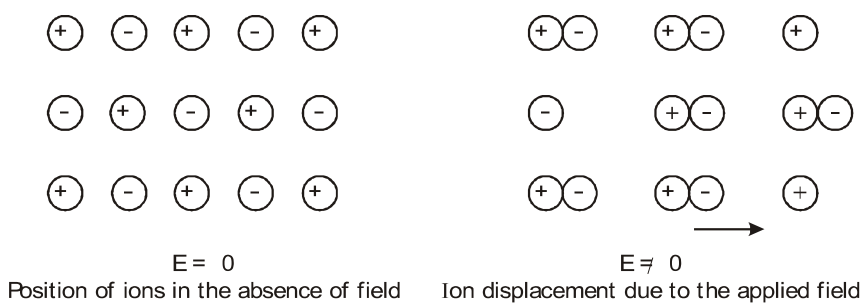


Fig. 8.4 Ionic Polarisation

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Expression for Ionic Polarisability a_i

Let an electric field E is applied to an ionic solid consisting of one cation and one anion per unit cell. This applied field causes the positive ions and negative ions to get displaced through a distance x_1 and x_2 respectively from their equilibrium position there by inducing a dipolemoment. Thus, the resultant dipolemoment per unit cell is

$$\mu = e\,(x_1 + x_2) \qquad ...(8.18)$$

Due to the application of electric field a restoring force is said to act over the cation and anion.

Thus,

Restoring force $\quad F = \beta_1 x_1 = \beta_2 x_2 \qquad ...(8.19)$

Hence, $\quad x_1 = \dfrac{F}{\beta_1}$ and $x_2 = \dfrac{F}{\beta_2} \qquad ...(8.20)$

where β_1 and β_2 are restoring force constants of cation and anion. This restoring force constants depends upon the mass of the ion and angular frequency of the molecule in which the ions are present.

Thus, $\quad x_1 = \dfrac{eE}{m\omega_o^2}$ and $x_2 = \dfrac{eE}{M\omega_o^2} \qquad ...(8.21)$

where m is the mass of cation and M the mass of anion.

Substituting equation (8.21) in (8.18), we get

$$\mu = e\left(\frac{eE}{m\omega_o^2} + \frac{eE}{M\omega_o^2}\right)$$

or

$$\mu = \frac{e^2 E}{\omega_o^2}\left(\frac{1}{m} + \frac{1}{M}\right) \qquad ...(8.22)$$

But, $\quad \mu = \alpha_i E \qquad ...(8.23)$

$\therefore$ Comparing equations (8.22) and (8.23) we get,

$$\alpha_i E = \frac{e^2 E}{\omega_o^2}\left(\frac{1}{m} + \frac{1}{M}\right)$$

or

$$\alpha_i = \frac{e^2}{\omega_o^2}\left(\frac{1}{m} + \frac{1}{M}\right). \qquad ...(8.24)$$

Thus, ionic polarisability is inversely propotional to the square of the natural frequency of the ionic molecule and directly proportional to its reduced mass.

The ionic polarisability is also independent of temperature.

3. Orientation Polarisation (Dipolar Polarisation)

Orientation polarisation occurs in dielectric materials which possess molecules with permanent dipole moment (i.e., in polar molecules).

In the absence of an external electric field, because of random orientation of the dipoles due to thermal agitation the material has net zero dipole moment. But, under the influence of an external applied electric field, each of the dipoles undergo rotation so as to reorient along the direction of the field as shown in figure 8.5. Thus, the material itself develops electrical polarisation.

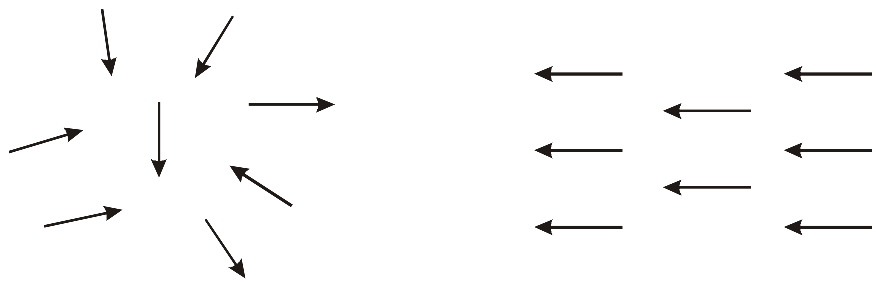


Fig. 8.5 *Orientation Polarisation*

This polarisation occur in ferroelectric materials such as BaTi O_3 and $PbTiO_3$ and produces a very high dielectric constant in these materials.

In the case of polar dielectrics, the orientational polarisability α_o is given by

$$\alpha_o = \frac{\mu^2}{3k_B T}$$

where k_B is the Boltzmann constant, T is the temperature and μ is the permanent dipole moment. Thus, the orientational polarisability is inversely proportional to absolute temperature.

4. Space Charge (Interfacial Polarisation)

The space charge polarisation occur in multiphase dielectric materials. When such materials are subjected to an external electric field, especially at high temperature the charges get accumulated at the interface or at the electrodes because of sudden change in conductivity as shown in Figure 8.8.

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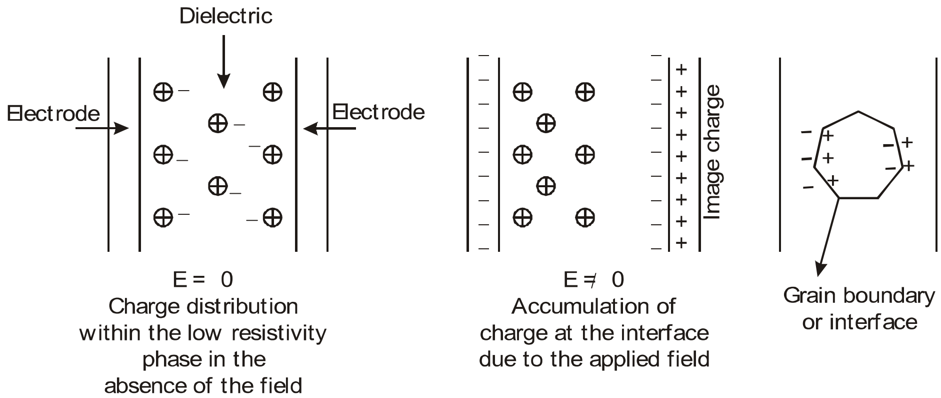


Fig. 8.6 *Space Charge Polarisation*

Since, the accumulation of charges with opposite polarity occurs at opposite parts in the low resistivity phase, it leads to the development of dipole moment within the low resistivity.

Grain boundaries often lead to interfacial polarisation as they can trap charges migrating under the influence of an applied field as shown in figure 8.8. This type of polarisation occur in some materials like $LiTaO_3$, $LiNbO_3$ and in certain glasses containing Li_2O or Na_2O. This polarisation is not an important factor in most common dielectrics used in capacitor and other applications.

Total Polarisability α_T

The total polarisability α_T of a material is thus given by the sum of the electronic, ionic and orientational polarisabilities.

$$\alpha_T = \alpha_e + \alpha_i + \alpha_o$$

Since, the space charge polarisability is very small when compared to other types of polarisabilities it is neglected.

Thus, the total polarisability of a material is given by

$$\alpha_T = 4\pi\varepsilon_o R^3 + \frac{e^2}{\omega_o{}^2}\left(\frac{1}{m}+\frac{1}{M}\right)+\frac{\mu^2}{3k_B T}$$

[Substituting for α_e, α_i and α_o]

Hence, the total polarisation P is given by

$$P = N\,\alpha_T\,E$$

or
$$P = NE\left[4\pi\varepsilon_o R^3 + \frac{e^2}{\omega_o{}^2}\left(\frac{1}{m}+\frac{1}{M}\right)+\frac{\mu^2}{3k_B T}\right]$$

The above equation is known as Langevin-Debye equation.

NOTES

Example 8.1

Copper is a Fcc crystal with a lattice constant 3.6 Å, and atomic number 29. If the average displacement of the electrons relative to the nucleus is 1×10^{-18} m on applying an electric field calculate the electronic polarisation.

Solution:

Given, $x = 1 \times 10^{-18}$ m; $a = 3.61 \times 10^{-10}$ m; Z = 29; P = ?

For Fcc crystal, number of atoms per unit cell is 4.

Number of electrons per m^3 =

$$\frac{(\text{Number of atoms / Unit cell})(\text{Number of electrons / Atom})}{a^3}$$

$$= \frac{4 \times 29}{(3.61 \times 10^{-10})^3} = \mathbf{2.465 \times 10^{30}\ electrons/m^3.}$$

Since, the electron density in copper is equal to the number of atoms per unit volume

N = 2.465×10^{30} atoms/m^3.

$$\therefore \quad P = N\mu$$

$$= N \times e \times x \qquad [\because \mu = ex)$$

$$= 2.465 \times 10^{30} \times 1.6 \times 10^{-19} \times 1 \times 10^{-18}$$

$$= 3.944 \times 10^{-7}\ C/m^2$$

$$\therefore \mathbf{P = 3.944 \times 10^{-7}\ C/m^2.}$$

Example 8.2

Silicon has a relative permittivity of 11.7 at frequencies high enough to ignore all but its electrical (optical) polarisability. It contains 4.82×10^{28} atoms/m^3. Calculate the dipole moment of each atom in a field of 10^4 Vm^{-1}, and also find the effective distance at this field strength between the center of the electron cloud in each atom and the nucleus.

Solution:

Given, $\varepsilon_r = 11.7$; N = 4.82×10^{28} atoms/m^3; μ = ?; x = ?

Formula $$\alpha_e = \frac{\varepsilon_o(\varepsilon_r - 1)}{N}$$

$$\alpha_e = \frac{8.85 \times 10^{-12}[11.7 - 1]}{4.82 \times 10^{28}} \qquad [\because \varepsilon_o = 8.85 \times 10^{-12}\ Fm^{-1}]$$

$$\boldsymbol{\alpha_e = 1.9646 \times 10^{-39}\ Fm^2.}$$

$$\because \quad \mu = \alpha_e E$$

$$= 1.9646 \times 10^{-39} \times 10^4$$

$$= 1.9646 \times 10^{-35}\ Cm^{-3}$$

NOTES

$\therefore \quad \boldsymbol{\mu = 1.9646 \times 10^{-35}\ Cm^{-3}.}$

Also,

$$\mu = Z\ e\ x$$

$$\therefore \quad x = \frac{\mu}{Ze} \qquad \text{(For silicon Z = 14)}$$

$$x = \frac{1.9646 \times 10^{-35}}{14 \times 1.6 \times 10^{-19}}$$

$$\therefore \quad \boldsymbol{x = 8.77 \times 10^{-18}\ m.}$$

$$\text{or} \quad \boldsymbol{x = 8.77 \times 10^{-8}\ Å.}$$

Example 8.3

Calculate the polarisability and relative permittivity in hydrogen gas with a density of 9.8×10^{26} atoms/m^3. Given the radius of the hydrogen atom to be 0.50 Å.

Solution:

Given, $N = 9.8 \times 10^{26}$ atoms/m^3; $R = 0.50 \times 10^{-10}$ m; α_e = ? and ε_r = ?

We know $\quad \alpha_e = 4\pi\varepsilon_o R^3$

$$= 4 \times 3.14 \times 8.85 \times 10^{-12} \times (0.50 \times 10^{-10})^3$$

$\therefore \quad \boldsymbol{\alpha_e =}$
1.389×10^{-41} Fm^2.

To find $\boldsymbol{\varepsilon_r}$ we know that,

$$\alpha_e = \frac{\varepsilon_o \times (\varepsilon_r - 1)}{N}$$

$$\text{or} \quad N\alpha_e = \varepsilon_o \times (\varepsilon_r - 1)$$

$$\frac{N\alpha_e}{\varepsilon_o} = \varepsilon_r - 1$$

$$\therefore \quad \varepsilon_r = \frac{N\alpha_e}{\varepsilon_o} + 1$$

$$\varepsilon_r = \frac{9.8 \times 10^{26} \times 1.389 \times 10^{-41}}{8.85 \times 10^{-12}} + 1$$

$$\varepsilon_r = 1.5381 \times 10^{-3} + 1$$

$$\therefore \quad \boldsymbol{\varepsilon_r = 1.0015.}$$

Example 8.4

The electronic polarisability of Argon atom is 1.75×10^{-40} Fm^2. What is the static dielectric constant of solid Argon, if its density is 1.8×10^3 kg/m^3 (given atomic weight of Ar = 39.95 and $N_A = 6.025 \times 10^{26}$/k mole).

Solution:

Given, α_e = 1.75 × 10^{-40} Fm^2; ρ = 1.8 × 10^3 kgm^{-3}; At. wt = 39.95; ε_r = ?

To find the number of atoms/unit volume

$$N = \frac{N_A \rho}{\text{At. wt}} = \frac{6.025 \times 10^{26} \times 1.8 \times 10^3}{39.95}$$

$$\therefore \quad \mathbf{N = 2.7146 \times 10^{28} \text{ atoms/m}^3.}$$

We know that,

$$\varepsilon_r = \frac{N\alpha_e}{\varepsilon_o} + 1$$

$$\varepsilon_r = \frac{2.7146 \times 10^{28} \times 1.75 \times 10^{-40}}{8.85 \times 10^{-12}} + 1$$

$$\varepsilon_r = 0.53679 + 1$$

$$\therefore \quad \boldsymbol{\varepsilon_r = 1.53679.}$$

5. Piezoelectricity

Piezoelectricity is the electric charge that accumulates in certain solid materials (such as, crystals, certain ceramics, and biological matter, such as bone, DNA and various proteins) in response to applied mechanical stress. The word piezoelectricity means electricity resulting from pressure and latent heat.

The piezoelectric effect results from the linear electromechanical interaction between the mechanical and electrical states in crystalline materials with no inversion symmetry. The piezoelectric effect is a reversible process: materials exhibiting the piezoelectric effect (the internal generation of electrical charge resulting from an applied mechanical force) also exhibit the reverse piezoelectric effect, the internal generation of a mechanical strain resulting from an applied electrical field. For example, lead zirconate titanate crystals will generate measurable piezoelectricity when their static structure is deformed by about 0.1% of the original dimension. Conversely, those same crystals will change about 0.1% of their static dimension when an external electric field is applied to the material. The inverse piezoelectric effect is used in the production of ultrasonic sound waves.

French physicists Jacques and Pierre Curie discovered piezoelectricity in 1880, and it has subsequently been exploited in a number of useful applications, such as the production and detection of sound, piezoelectric inkjet printing, generation of high voltages, clock generator in electronics, microbalances, to drive an ultrasonic nozzle, and ultrafine focusing of optical assemblies.

The nature of the piezoelectric effect is closely related to the occurrence of electric dipole moments in solids. The latter may either be induced for ions on crystal lattice sites with asymmetric charge surroundings (as in $BaTiO_3$ and PZTs) or may directly be carried by molecular groups (as in cane sugar). The dipole

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density or polarization (dimensionality [C•m/m^3]) may easily be calculated for crystals by summing up the dipole moments per volume of the crystallographic unit cell. As every dipole is a vector, the dipole density **P** is a vector field. Dipoles near each other tend to be aligned in regions called Weiss domains. The domains are usually randomly oriented, but can be aligned using the process of poling (not the same as magnetic poling), a process by which a strong electric field is applied across the material, usually at elevated temperatures. Not all piezoelectric materials can be poled.

Of decisive importance for the piezoelectric effect is the change of polarization **P** when applying a mechanical stress. This might either be caused by a reconfiguration of the dipole-inducing surrounding or by re-orientation of molecular dipole moments under the influence of the external stress. Piezoelectricity may then manifest in a variation of the polarization strength, its direction or both, with the details depending on the following:

1. Orientation of **P** within the Crystal
2. Crystal Symmetry
3. Applied Mechanical Stress

The change in **P** appears as a variation of surface charge density upon the crystal faces, i.e., as a variation of the electric field extending between the faces caused by a change in dipole density in the bulk. For example, a 1 cm^3 cube of quartz with 2 kN (500 lbf) of correctly applied force can produce a voltage of 12500 V.

Piezoelectric materials also show the opposite effect, called the converse piezoelectric effect, where the application of an electrical field creates mechanical deformation in the crystal.

8.4 PYRO AND FERRO ELECTRIC PROPERTIES OF CRYSTALS

Ferroelectricity refers to the creation of large induced dipole moment in a weak electric field as well as the existence of electric polarization even in the absence of an applied electric field.

Crystalline dielectric materials which possess a permanent electric polarization are called ferroelectric materials. Thus it is clear that, ferroelectric materials have electric dipole moment even in the absence of any field.

Examples: Barium Titanate ($BaTiO_3$), Potassium Dihydrogen Phosphate (KDP) (KH_2PO_4), Ammonium Dihydrogen Phosphate (ADP) ($NH_4H_2PO_4$).

Under the action of an external electric field, due to polarization of the material, an internal field gets created. The internal field increases and stabilizes the polarization. As a result, a part of polarization exists even if the field is removed.

Note:
- Ferroelectric, piezoelectric and pyroelectric materials are active dielectrics. i.e., these materials can be adapted to generate, modulate, amplify, convert electric signals and to store electrical energy when subjected to an external electric field. Only non-centrosymmetric crystals exhibit piezoelectic, pyroelectric and ferroelectric behaviour.
- **Piezoelectricity** : This term refers to the creation of electric potential by mechanical stress.
- **Pyroelectricity** : This term refers to the creation of electric potential by thermal stress.

Properties of Ferroelectric Materials

1. The ferroelectric materials exhibit domain structures similar to ferromagnetic materials.
2. These materials possess spontaneous polarization. But, the polarization P is not a linear function of applied field E . Hence these materials are known as non-linear dielectrics.
3 These materials exhibit ferroelectricity only when $T \leq T_C$. T_C is called the ferroelectric Curie temperature or transition temperature.
4. Ferroelecticity usually disappears above the transition temperature and the materials are converted to paraelectric materials. This shows that, above T_C the spontaneous polarization is destroyed by thermal disorder.
5. The condition for spontaneous polarization is given by $\frac{N\alpha_e}{3\varepsilon_0} = 1$.
6. Ferroelectric materials exhibit piezoelectricity and pyroelectricity.

Hysteresis

In ferroelectric materials, polarization P is not a linear function of applied electric field E. This is because, the relationship between P and E is complex in nature. In view of this, ferroelectrics are known as non-linear dielectrics. Such materials exhibit hysteresis curve similar to that of ferromagnetic materials. The hysteresis curve exhibited by a ferroelectric material is shown in Figure 8.7.

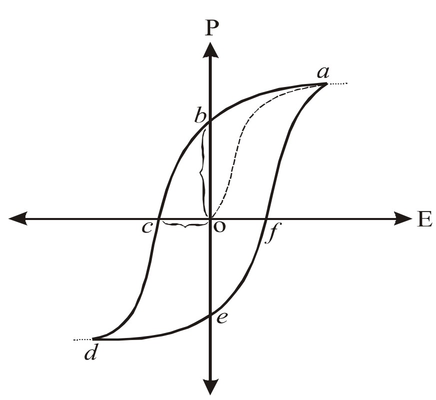


***Fig. 8.7** Ferroelectric hysteresis*

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Ferroelectric materials possess spontaneous polarization. Ferroelectricity is a result of dielectric hysteresis. *The lagging of polarization P behind the applied electric field E is called dielectric hysteresis.*

When an increasing electric field is applied to a ferroelectric material the relationship between P and E is shown by the line **oa**. As the value of E is increased continuously, the polarization attains a maximum and saturated value **a** as shown in Figure 8.14.

If now the applied electric field is reduced, the polarization also decreases from the point **a** , but fails to retrace the same path which it had while E was increasing.Thus the new path is **ab**. *But when E becomes zero a small amount of polarization exists in the material. This is known as residual polarization shown by the line* ob. Now the ferroelectric material is said to be spontaneously polarized. *In order to reduce the value of polarisation to zero, a reversing electric field* ***oc*** *should be applied. This field is known as coercive field.*

Further increase in E causes the specimen to get polarised in the opposite direction. This makes P also to increase in the opposite direction and reaches a saturation value again at **d**. Now also, when the field is decreased the curve traces the path **de** instead of **dc**.

Again the specimen gets completely depolarised at **f** when the direction of E is reversed and increased along OE. The curve traces the path up as E is increased further.

Thus, the variation of P *with respect to* E *traced along the closed path* **abcdefa** *in one full cycle of polarization and depolarization is called the hysteresis loop or the hysteresis curve.*

The area enclosed by the curve gives the energy loss per unit volume of the material per cycle.

Note:
- In ordinary dielectrics, the polarization P varies linearly with applied field E ($P = \chi \varepsilon_0 E$). Therefore, the ordinary dielectrics are often known as linear dielectrics.

Applications

1. Ferroelectric semiconductors such as $BaTiO_3$ - $SrTiO_3$, $BaTiO_3$ - $PbTiO_3$, $SrTiO_3$ - $PbTiO_3$ are used to make posistors. Posistors are the devices, which are used to measure and control temperature like thermistors.
2. Ferroelectric ceramics are used in the manufacture of capacitors to store electrical energy.
3. Piezoelectric materials are used to make pressure transducers, microphones and ultrasonic transducers.
4. Pyroelectric materials are used to make high sensitive infrared detectors.
5. Electrets (a type of ferroelectric material) are used in capacitors, microphones and gas filters to capture submicron particles by electrostatic attraction.

6. Electrets are also used as bandages over the fractured bones to speed up the healing process.
7. In optical communication, the ferroelectric crystals are used for optical modulation.

NOTES

Check Your Progress

1. Define the dielectric loss.
2. Elaborate on the dielectric breakdown.
3. Illustrate the thermal breakdown.
4. Explain the electrochemical breakdown.
5. What do you understand by the polarizability?
6. State the ionic polarisation.
7. Interpret the term ferroelectricity.
8. Define the dielectric hysteresis of ferroelectric materials.

8.5 ANSWERS TO CHECK YOUR PROGRESS QUESTIONS

1. Dielectric loss is a major problem involving heat generation and is dominating in high voltage application.
2. Whenever the voltage applied to a dielectric material exceeds a critical value a large amount of current flows through it. As a result of this, the dielectric loses its insulating property. This phenomena is known as dielectric breakdown.
3. When there is excessive increase in the temperature of the dielectric a local melting occurs due to less heat dissipation than heat generated. Hence, mobility of charge carriers is increased, and enormous current flows through the material thus, leading to thermal breakdown.
4. Dielectric breakdown due to the formation of electro chemical reaction or chemical reaction in a dielectric material is called electrochemical breakdown.
5. There are four different types of mechanisms through which electrical polarisation can occur in a dielectric material when they are subjected to an external electric field:
   - Electronic polarisation
   - Ionic polarisation
   - Orientation polarisation
   - Space charge or Interfacial polarisation

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6. Ionic polarisation occur only in ionic solids, such as NaCl which possess ionic bonds. It does not occur in covalent crystals such as diamond, silicon and germanium.
7. Ferroelectricity refers to the creation of large induced dipole moment in a weak electric field as well as the existence of electric polarization even in the absence of an applied electric field.
8. Ferroelectric materials possess spontaneous polarization. Ferroelectricity is a result of dielectric hysteresis. The lagging of polarization P behind the applied electric field E is called dielectric hysteresis.

8.6 SUMMARY

- Dielectric loss is a major problem involving heat generation and is dominating in high voltage application.
- The complementary angle $\delta = 90 - \theta$ is called the dielectric loss angle. This angle is a measure of the power or heat dissipated in each cycle. In most of the dielectrics this angle d is negligible.
- Whenever the voltage applied to a dielectric material exceeds a critical value a large amount of current flows through it. As a result of this, the dielectric loses its insulating property. This phenomena is known as dielectric breakdown.
- When there is excessive increase in the temperature of the dielectric a local melting occurs due to less heat dissipation than heat generated. Hence, mobility of charge carriers is increased, and enormous current flows through the material thus, leading to thermal breakdown
- Dielectric breakdown due to the formation of electro chemical reaction or chemical reaction in a dielectric material is called electrochemical breakdown.
- Discharge breakdown occurs due gaseous discharge taking place in occluded gas bubbles.
- The presence of cracks or pores at the surface of the material leads to defect breakdown due to the collection of moisture and other impurities at these defect sites.
- The electronic polarisation occurs, due to the displacement of the positively charged nucleus and the negatively charged electron cloud in opposite directions within a dielectric material upon applying an external electric field E.
- Ionic polarisation occur only in ionic solids, such as NaCl which possess ionic bonds. It does not occur in covalent crystals such as diamond, silicon and germanium.

- Orientation polarisation occurs in dielectric materials which possess molecules with permanent dipole moment (i.e., in polar molecules).
- The space charge polarisation occur in multiphase dielectric materials. When such materials are subjected to an external electric field, especially at high temperature the charges get accumulated at the interface or at the electrodes because of sudden change in conductivity.
- The piezoelectric effect results from the linear electromechanical interaction between the mechanical and electrical states in crystalline materials with no inversion symmetry.
- The piezoelectric effect is a reversible process: materials exhibiting the piezoelectric effect (the internal generation of electrical charge resulting from an applied mechanical force) also exhibit the reverse piezoelectric effect, the internal generation of a mechanical strain resulting from an applied electrical field.
- Ferroelectric materials possess spontaneous polarization. Ferroelectricity is a result of dielectric hysteresis. The lagging of polarization P behind the applied electric field E is called dielectric hysteresis.

NOTES

8.7 KEY WORDS

- **Dielectric loss:** Dielectric loss is a major problem involving heat generation and is dominating in high voltage application.
- **Dielectric breakdown:** Whenever the voltage applied to a dielectric material exceeds a critical value a large amount of current flows through it. As a result of this, the dielectric loses its insulating property. This phenomena is known as dielectric breakdown.
- **Discharge breakdown:** Discharge breakdown occurs due gaseous discharge taking place in occluded gas bubbles.
- **Ionic polarization:** Ionic polarisation occur only in ionic solids, such as NaCl which possess ionic bonds. It does not occur in covalent crystals, such as diamond, silicon and germanium.
- **Orientation polarization:** Orientation polarisation occurs in dielectric materials which possess molecules with permanent dipole moment (i.e., in polar molecules).
- **Space charge polarization:** The space charge polarisation occur in multiphase dielectric materials.

8.8 SELF ASSESSMENT QUESTIONS AND EXERCISES

NOTES

Short-Answer Questions

1. Explain the term dielectric loss.
2. Define about the dielectric breakdown.
3. Elaborate on the thermal breakdown.
4. Elucidate on the electrochemical breakdown.
5. What do you mean by the polarizability?
6. Interpret the ionic polarisation.
7. State the term ferroelectricity.
8. Explain the dielectric hysteresis of ferroelectric materials.

Long-Answer Questions

1. Briefly discuss the dielectric constant with the help of appropriate examples.
2. Differentiate between the dielectric breakdown and intrinsic breakdown.
3. Explain the polarizability on the basis of electronic, ionic and piezo.
4. Analyse the pyro and ferro electric properties of crystals. Give appropriate examples.

8.9 FURTHER READINGS

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BLOCK - III
MAGNETISM

NOTES

UNIT 9 PARAMAGNETISM

Structure

9.0 Introduction
9.1 Objectives
9.2 Classification of Magnetic Materials
9.3 Langevin's Theory of Paramagnetism
9.4 Quantum Theory of Paramagnetism
9.5 Answers to Check Your Progress Questions
9.6 Summary
9.7 Key Words
9.8 Self Assessment Questions and Exercises
9.9 Further Readings

9.0 INTRODUCTION

Paramagnetism is a form of magnetism whereby some materials are weakly attracted by an externally applied magnetic field, and form internal, induced magnetic fields in the direction of the applied magnetic field.

Paramagnetic materials include most chemical elements and some compounds; they have a relative magnetic permeability slightly greater than 1 (i.e., a small positive magnetic susceptibility) and hence are attracted to magnetic fields. The magnetic moment induced by the applied field is linear in the field strength and rather weak. It typically requires a sensitive analytical balance to detect the effect and modern measurements on paramagnetic materials are often conducted with a SQUID magnetometer.

Paramagnetism is due to the presence of unpaired electrons in the material, so most atoms with incompletely filled atomic orbitals are paramagnetic, although exceptions such as copper exist. Due to their spin, unpaired electrons have a magnetic dipole moment and act like tiny magnets. An external magnetic field causes the electrons' spins to align parallel to the field, causing a net attraction.

Materials that are called "Paramagnets" are most often those that exhibit, at least over an appreciable temperature range, magnetic susceptibilities that adhere to the Curie or Curie–Weiss laws. In principle any system that contains atoms,

ions, or molecules with unpaired spins can be called a paramagnet, but the interactions between them need to be carefully considered.

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Paramagnets do not retain any magnetization in the absence of an externally applied magnetic field because thermal motion randomizes the spin orientations. Some paramagnetic materials retain spin disorder even at absolute zero, meaning they are paramagnetic in the ground state, i.e. in the absence of thermal motion.

In this unit, you will study about the classification of magnetic materials, Langevin's theory of paramagnetism, and quantum theory of paramagnetism.

9.1 OBJECTIVES

After going through this unit, you will be able to:

- Define the classification of magnetic materials
- Explain the Langevin's theory of paramagnetism
- Comprehend the quantum theory of paramagnetism

9.2 CLASSIFICATION OF MAGNETIC MATERIALS

Magnetic materials are classified into different categories based on their magnetic parameters (like χ and μ_r) and their microscopic magnetic structure under different environmental conditions (i.e., under the influence of magnetic field, temperature etc.).

Based on whether the atoms carry permanent magnetic dipoles or not, and also on the basis of effect of temperature and magnetic field on the magnetic properties; all materials are classified broadly into the following three categories.

1. Diamagnetic materials,
2. paramagnetic materials, and
3. ferromagnetic materials.

Two more classes of materials have structure very close to ferromagnetic materials but possess quite different magnetic effects. They are:

4. antiferromagnetic materials, and
5. ferrimagnetic materials.

Materials which lack permanent dipoles are called diamagnetic.

If the atoms or molecules of a material have permanent dipoles, such a material may be paramagnetic,ferromagnetic,antiferromagnetic or ferrimagnetic, depending on the interaction between the individual dipoles.

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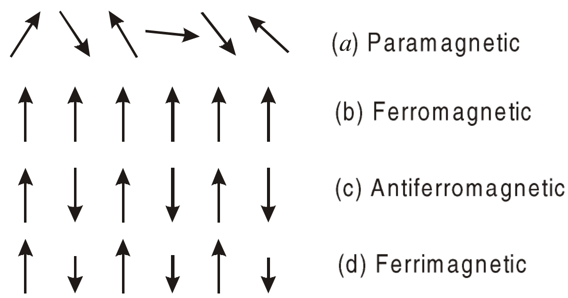


Fig. 9.1 *Illustration of Arrangement of Permanent Magnetic Dipoles in a Paramagnetic, Ferromagnetic, Antiferromagnetic and Ferrimagnetic Material*

If the interaction between the permanent dipoles is either negligible or if they do not interact among themselves as shown in Figure 9.1(*a*), the materials is paramagnetic.

If the magnetic dipoles interact in such a way they tend to orient in the same direction as shown in Figure 9.1(*b*), the material is ferromagnetic.

If the neighbouring dipoles orient in opposite directions and if the dipoles are of equal magnitude as shown in Figure 9.1(*c*), the materials is antiferromagnetic.

On the otherhand, if the neighbouring dipoles are of different magnitude and orient themselves in anti-parallel direction as shown in Figure 9.1(*d*), then the material is ferrimagnetic.

Summary of Classification of Magnetic Materials on the Basis of Orientation of Dipoles

Classification	Permanent dioples	Interaction between neighbouring dipoles
Diamagnetic	Absent	—
Paramagnetic	Present	Negligible.
Ferromagnetic	Present	Parallel orientation.
Antiferromagnetic	Present	Anti-parallel orientation of equal magnitude.
Ferrimagnetic	Present	Anti-parallel orientation of unequal magnitude.

It has been observed through many studies in the past that electrons revolve around the nucleus in circular orbits. A moving electron can be considered as an electric current whereas it also demonstrates a magnetic dipole moment normal to the plane in which the electron is orbiting. As the direction of the revolution of an electron flips the direction of the magnetic moment also turns in the opposite direction. Now, according to Langevin’s theory, the paired electrons in the atoms of a diamagnetic substance revolve in such a way that the magnetic moments caused

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by them cancel out each other. As a result, no net magnetic moment is obtained by the orbital motion of the electrons. Therefore, it can be stated that all electrons are paired in an atom of a diamagnetic material. When a magnetic field is applied perpendicular to the plane of the orbiting electron, the angular velocity of the revolving electron would change without any change in the radius. The change in the angular velocity will depend upon the direction of the magnetic field. The variation in the angular velocity causes a variation in the magnetic moment of the atom.

9.3 LANGEVIN'S THEORY OF PARAMAGNETISM

All materials are inherently diamagnetic. The orbital motion of electrons create tiny atomic current loops, which produce magnetic field. Under such a condition, when an external magnetic field is applied to a material, these current loops will tend to align in such a way as to oppose the applied field.

Thus diamagnetism can be viewed as, the result of Lenz`s law, i.e., an induced magnetic field tend to oppose the change which created it.

Diamagnetism occurs in substances whose atom consists of an even number of electrons. The electrons of such atoms are paired. The electrons in each pair have orbital motion as well as spin motions in opposite sense. Thus, the resultant magnetic dipole moment is zero.

General Properties of Diamagnetic Materials

1. Diamagnetic materials experience a repelling force when brought near the pole of a strong magnet.
2. In a non-uniform magnetic field, they are repelled away from stronger parts of the field.
3. These materials do not retain the magnetic properties when the external field is removed.
4. The magnetic susceptibility χ of these materials is always negative.
5. The relative permeability μ_r is always less than one (i.e., $\mu_r < 1$).
6. In the absence of an external magnetic field, the net magnetic dipole moment over each atom or molecule of a diamagnetic material is zero. This is due to the pairing of electrons.
7. Both susceptibility and relative permeability are independent of applied magnetic field and temperature.
8. **Examples**: Bismuth, copper, lead, zinc and rare gases.

9.4 QUANTUM THEORY OF PARAMAGNETISM

Paramagnetism is a result of the presence of some unpaired electrons and from the realignment of the electron orbits caused by the external magnetic

field. In paramagnetic materials, the magnetic fields due to the orbiting and spinning electrons do not cancel out. Thus there will be a net intrinsic moment.

General Properties of Paramagnetic Materials

NOTES

1. Paramagnetic materials experience a feeble attractive force when brought near the pole of a magnet.
2. They are attracted towards the stronger parts of an inhomogeneous magnetic field.
3. These materials possess some permanent dipole moment which arise due to some unpaired electrons.
4. In the absence of an external magnetic field, the dipoles are randomly oriented. Thus the net magnetization is zero.
5. When these materials are placed in an external magnetic field, realignment of the electron orbits and magnetic dipoles take place resulting in a small magnetization.
6. These materials do not retain the magnetic properties when the external field is removed.
7. The magnetic susceptibility χ is small and positive.
8. The permeability is slightly greater than one (i.e., $\mu_r > 1$).

   It is given by, $\chi = \frac{C}{T - \theta}$ where C is the Curie`s constant, T is the absolute temperature and θ is Curie temperature.
9. When the temperature is less than Curie temperature, paramagnetic materials become diamagnetic material.
10. **Examples**: Platinum, aluminium, copper sulphate, magenese sulphate and the salts of iron and nickel.

Check Your Progress

1. Explain the classification of magnetic materials.
2. Define the Langevin's theory of paramagnetism.
3. Illustrate the quantum theory of paramagnetism.
4. State the general properties of paramagnetic materials.

9.5 ANSWERS TO CHECK YOUR PROGRESS QUESTIONS

1. Magnetic materials are classified into different categories based on their magnetic parameters (like χ and μ_r) and their microscopic magnetic structure

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under different and their microscopic magnetic structure under different environmental conditions (i.e., under the influence of magnetic field, temperature, etc.).

2. All materials are inherently diamagnetic. The orbital motion of electrons create tiny atomic current loops, which produce magnetic field. Under such a condition, when an external magnetic field is applied to a material, these current loops will tend to align in such a way as to oppose the applied field.
3. Paramagnetism is a result of the presence of some unpaired electrons and from the realignment of the electron orbits caused by the external magnetic field. In paramagnetic materials, the magnetic fields due to the orbiting and spinning electrons do not cancel out. Thus there will be a net intrinsic moment.
4. Paramagnetic materials experience a feeble attractive force when brought near the pole of a magnet. They are attracted towards the stronger parts of an inhomogeneous magnetic field.

9.6 SUMMARY

- Magnetic materials are classified into different categories based on their magnetic parameters (like χ and μ_r) and their microscopic magnetic structure under different and their microscopic magnetic structure under different environmental conditions (i.e., under the influence of magnetic field, temperature, etc.).
- All materials are inherently diamagnetic. The orbital motion of electrons create tiny atomic current loops, which produce magnetic field. Under such a condition, when an external magnetic field is applied to a material, these current loops will tend to align in such a way as to oppose the applied field.
- Diamagnetism occurs in substances whose atom consists of an even number of electrons. The electrons of such atoms are paired. The electrons in each pair have orbital motion as well as spin motions in opposite sense. Thus, the resultant magnetic dipole moment is zero.
- Paramagnetism is a result of the presence of some unpaired electrons and from the realignment of the electron orbits caused by the external magnetic field. In paramagnetic materials, the magnetic fields due to the orbiting and spinning electrons do not cancel out. Thus there will be a net intrinsic moment.
- Paramagnetic materials experience a feeble attractive force when brought near the pole of a magnet. They are attracted towards the stronger parts of an inhomogeneous magnetic field.

9.7 KEY WORDS

NOTES

- **Classification of magnetic materials:** Magnetic materials are classified into different categories based on their magnetic parameters (like χ and μ_r) and their microscopic magnetic structure under different and their microscopic magnetic structure under different environmental conditions (i.e., under the influence of magnetic field, temperature, etc.).
- **Langevin's theory of paramagnetism:** All materials are inherently diamagnetic. The orbital motion of electrons create tiny atomic current loops, which produce magnetic field. Under such a condition, when an external magnetic field is applied to a material, these current loops will tend to align in such a way as to oppose the applied field.
- **Quantum theory of paramagnetism:** Paramagnetism is a result of the presence of some unpaired electrons and from the realignment of the electron orbits caused by the external magnetic field. In paramagnetic materials, the magnetic fields due to the orbiting and spinning electrons do not cancel out. Thus there will be a net intrinsic moment.

9.8 SELF ASSESSMENT QUESTIONS AND EXERCISES

Short-Answer Questions

1. Define the classification of magnetic materials.
2. State the Langevin's theory of paramagnetism.
3. Explain the quantum theory of paramagnetism.
4. Interpret the general properties of paramagnetic materials.

Long-Answer Questions

1. Discuss the classification of magnetic materials. Give appropriate examples.
2. Analyse the Langevin's theory of paramagnetism.
3. Explain the quantum theory of paramagnetism.

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UNIT 10 FERROMAGNETISM

NOTES

Structure

10.0 Introduction
10.1 Objectives
10.2 Ferromagnetism
10.3 Weiss Molecular Field Theory
10.4 Ferromagnetism Domains
10.5 Answers to Check Your Progress Questions
10.6 Summary
10.7 Key Words
10.8 Self Assessment Questions and Exercises
10.9 Further Readings

10.0 INTRODUCTION

Ferromagnetism is the strongest type and is responsible for the common phenomenon of magnetism in magnets encountered in everyday life. Ferromagnetism is the basic mechanism by which certain materials (such as iron) form permanent magnets, or are attracted to magnets. In physics, several different types of magnetism are distinguished.

Ferromagnetism is very important in industry and modern technology, and is the basis for many electrical and electromechanical devices such as electromagnets, electric motors, generators, transformers, and magnetic storage such as tape recorders, and hard disks, and non-destructive testing of ferrous materials. Permanent magnets (materials that can be magnetized by an external magnetic field and remain magnetized after the external field is removed) are either ferromagnetic or ferromagnetic, as are the materials that are noticeably attracted to them. Only a few substances are ferromagnetic. The common ones are iron, cobalt, nickel and most of their alloys, and some compounds of rare earth metals.

Ferromagnetic materials can be divided into magnetically "Soft" materials like annealed iron, which can be magnetized but do not tend to stay magnetized, and magnetically "Hard" materials, which do. Permanent magnets are made from "Hard" ferromagnetic materials such as alnico, and ferromagnetic materials such as ferrite that are subjected to special processing in a strong magnetic field during manufacture to align their internal microcrystalline structure, making them very hard to demagnetize.

Ferromagnetism is an unusual property that occurs in only a few substances. The common ones are the transition metals iron, nickel, cobalt and their alloys, and alloys of rare earth metals. It is a property not just of the chemical make-up of a material, but of its crystalline structure and microstructure. There are ferromagnetic metal alloys whose constituents are not themselves ferromagnetic, called Heusler alloys, named after Fritz Heusler.

In this unit, you will study about the ferromagnetism, the Weiss molecular field theory, and the ferromagnetic domains.

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10.1 OBJECTIVES

After going through this unit, you will be able to:

- Understand the ferromagnetism
- Explain the Weiss molecular field theory
- Interpret the ferromagnetic domains

10.2 FERROMAGNETISM

Ferromagnetism is a phenomenon in which a material gets magnetized to a very large extent in the presence of an external field. The direction in which the material gets magnetized is the same as that of the external field.

Further, *these materials exhibit magnetization even in the absence of an external magnetic field. This property is called spontaneous magnetization*.

General Properties of Ferromagnetic Materials

1. The atoms or molecules of ferromagnetic materials have a net intrinsic magnetic dipole moment due to the spin of the electrons. So they act as strong magnets.
2. Ferromagnetic materials experience a very strong attractive force when brought near the pole of a magnet.
3. When a ferromagnetic material is subjected to the influence of a magnetic field, all magnetic lines of force pass through it.
4. These materials exhibit high degree of magnetization and get permanently magnetized. i.e., they will continue to retain the magnetic property even when the external field is removed. This property is called spontaneous magnetization.
5. Permeability is very much greater than one (i.e., $\mu_r >> 1$).
6. Susceptibility is positive and high. It is given by $\chi = \frac{C}{T - \theta}$ which is called the Curie- Weiss law. C is the Curie constant, T is the absolute temperature and θ is the ferromagnetic Curie temperature. When $T < \theta$, the material is in ferromagnetic state.
7. When $T > \theta$, ferromagnetic materials behave like an ordinary paramagnetic material. The variation of χ with temperature is shown in Figure 10.1.

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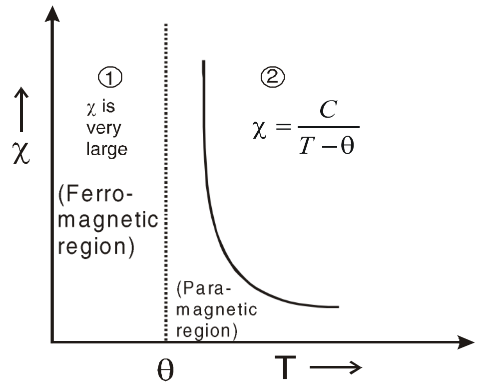


Fig. 10.1 *Variation of the Susceptibility with Temperature in a Ferromagnetic Material*

8. **Examples**: Fe, Co,Ni, Fe_3O_4, MnAs, gadolinium, etc.

10.3 WEISS MOLECULAR FIELD THEORY

Pierre-Ernest Weiss (25 March 1865, Mulhouse – 24 October 1940, Lyon) was a French physicist specialized in magnetism. He developed the domain theory of ferromagnetism in 1907. Weiss also developed the molecular or mean field theory, which is often called Weiss-mean-field theory, which lead to the discovery of the Curie-Weiss law.

According to Weiss, in a real gas, the molecules are mutually influenced by their magnetic moments and consequently, there should exist a molecular field, within the gas. This field, produced at any point by all the neighbouring molecules, is proportional to the same logic as the intensity of magnetization. Let this internal molecular field be represented by H_i. Then,

$$H_i = \lambda M$$

Here, λ is molecular field coefficient. M is the magnetization.

Then, the effecting field is,

$$H_e = H + H_i = H + \lambda M$$

According to Langevin's theory of paramagnetism,

$$M = nm^2 \mu_0 H / 3KT = \mu_0 M^2_s H/3nkT$$

m = Magnetic moment of each atoms.

n = Number of atoms per unit volume.

H = Magnetic field intensity.

K = Boltzmann's constant.

T = Absolute temperature.

$M_s = nm$ = Saturation value of magnetization.

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Weiss replaced H by H_e. Therefore,

$$M = \mu_0 M_s^2 (H + \lambda M) / 3nkT \quad ...10.1$$

Now,

Volume susceptibility $\chi_m = M/H = \mu_0 nm^2 (H + \lambda M)/3kTH$

i.e., $\chi_m = \mu_0 nm^2 /3kT = + \lambda\mu_0 nm^2 /2kT \chi_m$

Or $\chi_m = (1 - \lambda \mu_0 nm^2 /2kT) = \mu_0 nm^2 /3kT$

$$\chi_m = (\mu_0 nm^2 /3kT) = (\mu_0 nm^2 /3k) / T - \lambda \mu_0 nm^2 /(T - \lambda \mu_0 nm^2 /3k) = C/T - \theta \quad ...10.2$$

Equation 10.2 is known as Curie-Weiss law. The constant θ is known as Curie temperature. Curie-Weiss law shows that below Curie temperature ($T < \theta$), susceptibility becomes negative. However, it should be noted that for most of the paramagnetic substances, Curie temperature is quite low so that a situation for which $T < \theta$ is rare.

Langevin's theory of paramagnetism was modified by Weiss through introducing the concept of internal fields. Weiss supposed that in a real gas, the molecules influence each other via their magnetic moments. A molecular field should exist within the gas. This field at any point, contributed by all the coordinating molecules, is directly proportional to the intensity of magnetization.

At that time, Weiss also introduced a theoretical concept of ferromagnetic domains. The atoms of the ferromagnetic material align in the same direction in a small region due to certain mutual exchange interaction. It was named as a domain. Therefore, Weiss's theory of ferromagnetism is also known as domain theory of ferromagnetism. Some main points of this theory are the following:

(1) The size of the domains aligned fairly along the direction of the applied magnetic field at the cost of the domains oriented in another direction. The domains aligned opposite to the applied field get reduced. Overall, the domain boundaries (also known as domain walls) move to expand the domain in a favorable orientation.

(2) Likewise, domains rotate and orient themselves along the external magnetic field. When a weak external field is applied, the process of magnetization in the material happens mostly because of the growing domain, however, in the case of a strong magnetic field, the material is mostly magnetized through domain alignment. After that when the field is removed, the domain walls do not get back their original positions, therefore, the material is not demagnetized completely. Some residual magnetism remains in this. Thereafter, in 1907, Weiss postulated molecular field theory to deduce the prominent features of ferromagnetism.

10.4 FERROMAGNETISM DOMAINS

The magnetization and hysteresis observed in a ferromagnetic material is explained using the concept of domain proposed by Weiss in 1907.

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According to this domain concept, a specimen of ferromagnetic material consists of different region which are spontaneously magnetised below the Curie temperature. *These spontaneously magnetised or self magnetised regions in a ferromagnetic material is called domains*. Each domain is separated by the other domain by domain walls which has finite dimension.

At finite temperature ($T< T_c$), and in the absence of an external magnetic field, the direction of magnetization of each domain have random orientation in space as shown in Figure10.2.

Because of this randomness, the resultant magnetic moment of the material as a whole (which is the vectorial sum of the magnetic moment of the constituent domains) turn out to be zero.

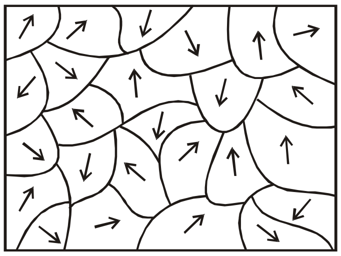


Fig. 10.2 *Random Orientation of Magnetic Moments of the Domains*

Effect of External Magnetic Field on The Domains

A symbolic representation of the response of the domains to the magnetic field is shown in Figure 10.3. In the absence of an external magnetic field the relative orientation of the magnetic moments of various domains will be completely random as shown in Figure 10.3(*a*).

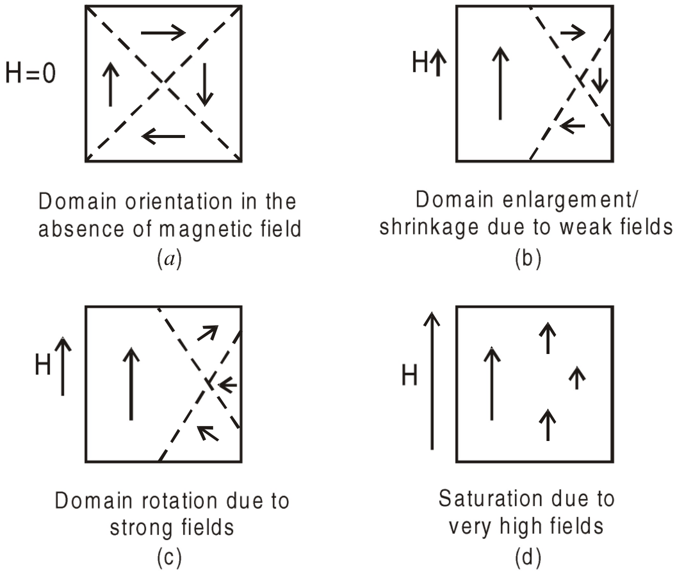


Fig. 10.3 *Domain Response to the Field*

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When an external magnetic field is applied, depending on the strength of the applied magnetic field, the magnetization effect may take place in any one of the following three stages.

1. Due to domain wall movement or
2. Due to the rotation of domains magnetic moments and
3. Due to both of the above two process.

1. When the applied field is weak, the domains which have their resultant magnetic moments in a direction parallel to (atleast favourably oriented to) the direction of the applied field expand their size at the cost of other domains with unfavourably oriented magnetic moments. Thus the domain areas of unfavourably oriented magnetic moments diminish (Figure 10.3(*b*)) thereby providing a large net magnetization.
2. When the field becomes strong, the domain's magnetic moments rotate partially and tend to align in the direction of the magnetic field (Figure 10.3(*c*)). This results in further increase in the magnetization of the material.
3. When the field become very strong, the magnetic moments of each and every domain undergo required amount of rotation so as to align perfectly along the direction of the field (Figure 10.3(*d*)). *This indicates the ultimate stage of magnetization. This state of magnetization is called saturation.* Beyond this saturation stage, further increase in magnetization is impossible, no matter how strong the field is.

Check Your Progress

1. What do you understand by the ferromagnetism?
2. Explain the general properties of ferromagnetic materials.
3. Define the Weiss molecular field theory.
4. Elaborate on the ferromagnetism domains.
5. Illustrate the effect of external magnetic field on the domains.

10.5 ANSWERS TO CHECK YOUR PROGRESS QUESTIONS

1. Ferromagnetism is a phenomenon in which a material gets magnetized to a very large extent in the presence of an external field. The direction in which the material gets magnetized is the same as that of the external field.
2. Ferromagnetic materials experience a very strong attractive force when brought near the pole of a magnet. When a ferromagnetic material is subjected to the influence of a magnetic field, all magnetic lines of force pass through it.

3. According to Weiss, in a real gas, the molecules are mutually influenced by their magnetic moments and consequently, there should exist a molecular field, within the gas. This field, produced at any point by all the neighbouring molecules, is proportional to the same logic as the intensity of magnetization.
4. According to domain concept, a specimen of ferromagnetic material consists of different region which are spontaneously magnetised below the Curie temperature. These spontaneously magnetised or self -magnetised regions in a ferromagnetic material is called domains.
5. In the absence of an external magnetic field the relative orientation of the magnetic moments of various domains will be completely random. When an external magnetic field is applied, depending on the strength of the applied magnetic field, the magnetization effect may take place in different kind of stages.

NOTES

10.6 SUMMARY

- Ferromagnetism is a phenomenon in which a material gets magnetized to a very large extent in the presence of an external field. The direction in which the material gets magnetized is the same as that of the external field.
- These materials exhibit magnetization even in the absence of an external magnetic field. This property is called spontaneous magnetization.
- Ferromagnetic materials experience a very strong attractive force when brought near the pole of a magnet. When a ferromagnetic material is subjected to the influence of a magnetic field, all magnetic lines of force pass through it.
- Pierre-Ernest Weiss (25 March 1865, Mulhouse – 24 October 1940, Lyon) was a French physicist specialized in magnetism. He developed the domain theory of ferromagnetism in 1907. Weiss also developed the molecular or mean field theory, which is often called Weiss-mean-field theory.
- According to Weiss, in a real gas, the molecules are mutually influenced by their magnetic moments and consequently, there should exist a molecular field, within the gas. This field, produced at any point by all the neighbouring molecules, is proportional to the same logic as the intensity of magnetization.
- According to domain concept, a specimen of ferromagnetic material consists of different region which are spontaneously magnetised below the Curie temperature. These spontaneously magnetised or self -magnetised regions in a ferromagnetic material is called domains.
- In the absence of an external magnetic field the relative orientation of the magnetic moments of various domains will be completely random. When an external magnetic field is applied, depending on the strength of the applied magnetic field, the magnetization effect may take place in different kind of stages.

NOTES

10.7 KEY WORDS

- **Ferromagnetism:** Ferromagnetism is a phenomenon in which a material gets magnetized to a very large extent in the presence of an external field.
- **Weiss molecular field theory:** According to Weiss, in a real gas, the molecules are mutually influenced by their magnetic moments and consequently, there should exist a molecular field, within the gas.
- **Ferromagnetism domains:** According to domain concept, a specimen of ferromagnetic material consists of different region which are spontaneously magnetised below the Curie temperature.

10.8 SELF ASSESSMENT QUESTIONS AND EXERCISES

Short-Answer Questions

1. Elaborate on the ferromagnetism.
2. Define the general properties of ferromagnetic materials.
3. State the Weiss molecular field theory.
4. Explain the ferromagnetism domains.
5. Interpret the effect of external magnetic field on the domains.

Long-Answer Questions

1. Briefly describe the ferromagnetism with the help of examples.
2. Analyse the Weiss molecular field theory.
3. Discuss the ferromagnetism domains.

10.9 FURTHER READINGS

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UNIT 11 ANTIFERROMAGNETISM AND FERRIMAGNETISM

NOTES

Structure

11.0 Introduction
11.1 Objectives
11.2 Antiferromagnetism
11.3 Neel's Theory
11.4 Ferrimagnetism and Ferrites
11.5 Answers to Check Your Progress Questions
11.6 Summary
11.7 Key Words
11.8 Self Assessment Questions and Exercises
11.9 Further Readings

11.0 INTRODUCTION

Antiferromagnetism plays a crucial role in giant magnetoresistance, as had been discovered in 1988 by the Nobel prize winners Albert Fert and Peter Grünberg (awarded in 2007) using synthetic antiferromagnets. In materials that exhibit antiferromagnetism, the magnetic moments of atoms or molecules, usually related to the spins of electrons, align in a regular pattern with neighbouring spins (on different sub lattices) pointing in opposite directions. This is, like ferromagnetism and ferrimagnetism, a manifestation of ordered magnetism.

Antiferromagnetic materials occur commonly among transition metal compounds, especially oxides. Examples include hematite, metals, such as chromium, alloys, such as iron manganese (FeMn), and oxides, such as nickel oxide (NiO). There are also numerous examples among high nuclearity metal clusters. Organic molecules can also exhibit antiferromagnetic coupling under rare circumstances, as seen in radicals, such as 5-dehydro-*m*-xylylene.

Generally, antiferromagnetic order may exist at sufficiently low temperatures, but vanishes at and above the Neel temperature – named after Louis Neel, who had first identified this type of magnetic ordering. Above the Neel temperature, the material is typically paramagnetic.

Antiferromagnetic structures were first shown through neutron diffraction of transition metal oxides, such as nickel, iron, and manganese oxides. The experiments, performed by Clifford Shull, gave the first results showing that magnetic dipoles could be oriented in an antiferromagnetic structure.

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A ferrimagnetic material is material that has populations of atoms with opposing magnetic moments, as in antiferromagnetism. For ferrimagnetic materials these moments are unequal in magnitude so a spontaneous magnetization remains. This can for example happen when the populations consist out of different atoms or ions (such as, Fe^{2+} and Fe^{3+}).

Ferrimagnetism has the same physical origins as ferromagnetism and antiferromagnetism. In ferrimagnetic materials the magnetization is also caused by a combination of dipole-dipole interactions and exchange interactions resulting from the Pauli exclusion principle. The main difference is that in ferrimagnetic materials there are different types of atoms in the material's unit cell.

Ferrimagnetism has often been confused with ferromagnetism. The oldest known magnetic substance magnetite (Fe_3O_4) was classified as a ferromagnet before Louis Neel discovered ferrimagnetism in 1948. Since the discovery, numerous uses have been found for ferrimagnetic materials, such as hard drive platters and biomedical applications.

In this unit, you will study about the antiferromagnetism, the Neel's theory, the ferrimagnetism, and the ferrites.

11.1 OBJECTIVES

After going through this unit, you will be able to:

- Comprehend the antiferromagnetism
- Understand the Neel's theory
- Elaborate on the ferrimagnetism
- Define what ferrites are

11.2 ANTIFERROMAGNETISM

Antiferromagnetism refers to a phenomenon in which the magnetic interaction between any two dipoles align themselves anti-parallel to each other. Since all the dipoles are of equal magnitude, the net magnetization is zero.

General Properties of Antiferromagnetic Materials

1. Like ferromagnetic materials antiferromagnetic materials also possess dipole moment due to spin of the electron.
2. The magnetic interaction between any two dipoles align themselves anti-parallel to each other. Since all the dipoles are equal in magnitude and due to anti-parallel alignment, the resultant magnetic effect is zero.
3. The opposite alignment of adjacent dipoles is due to an exchange interaction.

4. These materials have a temperature dependent magnetism due to the distruption of the magnetic moment alignment.
5. The susceptibility is very small and is positive. It is given by $\chi = \frac{C}{T+\theta}$ for $T > T_N$, where T_N is the Neel temperature. C is the Curie constant and θ the paramagnetic Curie temperature.
6. Initially, the susceptibility increases slightly as temperature increases and beyond a particular temperature known as Neel temperature, the susceptibility decreases with temperature as shown in Figure 11.1.

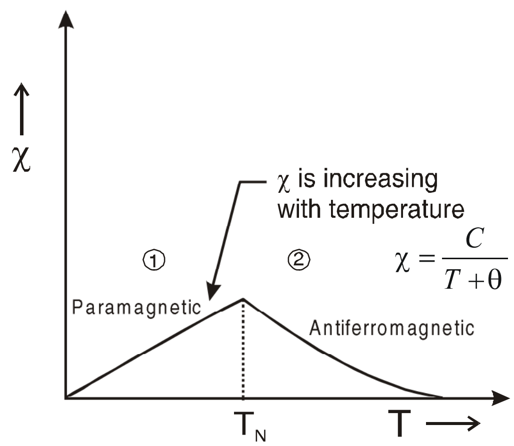


Fig. 11.1 *Variation of the Susceptibility with Termperature in Antiferromagnetic Material*

7. **Examples:** Ferrous oxide (FeO), magenese oxide (MnO), chromium oxide (Cr_2O_3), copper chloride ($CuCl_2$), FeF_2, Nd, Eu; etc.

11.3 NEEL'S THEORY

In 1949 French physicist Louis Neel (1904-2000) discovered that when they are finely divided, ferromagnetic nanoparticles lose their hysteresis below a certain size; this phenomenon is known as superparamagnetism. The magnetization of these materials is subject to the applied field, which is highly non-linear.

This curve is well described by the Langevin function, but for weak fields it can be simply written as:

$$M(H) = \chi_0 H + N_e H^3 + \varepsilon(H^3),$$

Where χ_0 is the susceptibility at zero field and N_e is known as the Neel coefficient. The Neel coefficient reflects the non-linearity of superparamagnetic materials in low fields.

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We can express this theory as following:

If a coil of N turns with a surface S through which passes a current of excitation I_{exc} is immersed in a magnetic field H_{ext} collinear with the axis of the coil, a superparamagnetic material is deposited inside the coil.

The electromotive force to the terminals of a winding of the coil, e, is given by the formula:

$$e = -d\phi/dt = -SdB/dt$$

Where B is the magnetic induction given by the equation,

$$B = \mu_0 \mu_r (H + M)$$

In the absence of magnetic material,

$$M = 0$$

And

$$B = \mu_0 \mu_r (H_{ext} + H_{\text{exc}}).$$

Differentiating this expression, the frequency of the voltage is the same as the excitation current i_{exc} or the magnetic field H_{ext}.

In the presence of superparamagnetic material, neglecting the higher terms of the Taylor expansion, we obtain for *B*:

$$B = \mu_0 \mu_r ((1 + \chi_0)(H_{ext} + H_{\text{exc}}) + N_e (H_{ext} + H_{\text{exc}})^3).$$

The Néel theory of ferrimagnetism is a molecular-field theory of magnetic ordering in systems which contain non-equivalent substructures of magnetic ions. Following are the two principal results of the theory:

(a) The curve of reciprocal susceptibility vs temperature above the Curie temperature is a hyperbola.

(b) The curve of spontaneous magnetization vs temperature below the Curie temperature may have any one of a number of unusual forms.

The exact form depends on the distribution of magnetic ions between the substructures and on the relative values of the molecular field coefficients.

The Néel temperature is defined as the Curie point of antiferromagnetic in honour of the French physicist Louis Néel. Antiferromagnetism is successfully explained by him in 1936. This extemporaneous antiparallel coupling of atomic magnets is interrupted by heating and distribute completely above a specified temperature, defined as Néel temperature. It is the characteristic of every antiferromagnetic material. Few antiferromagnetic materials have this temperature at several hundred degrees more than the room temperature. Generally, these temperatures for materials are lower. For manganese oxide, Néel temperature is 122 K (–240° F, or –151° C).

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In an external applied magnetic field, antiferromagnetic solids have specific behaviour which depends upon the temperature. These solids do not respond to the external field at very low temperatures, because the antiparallel arrangement of the atomic magnets is firmly maintained. When the temperature increases, some atoms break free of the even arrangement and align themselves with the external field. This alignment and the delicate magnetism which it is used to produces in the solid reach their highest value at the Néel temperature. When it crosses the Neel temperature alignment of the atoms with the magnetic field is gradually prevented by thermal agitation. So, as the temperature is increased the weak magnetism which is produced in the solids through the alignment of its atoms decreases continuously.

Magnets have many uses in regular life. Examples of hard magnets are magnets on the refrigerator and magnetic strips on the back of credit cards. Hard magnets maintain their magnetism easily as compared to the other magnets and are therefore very useful in the applications of data memory. Magnetic materials have different degrees of magnetism naturally which are characterized by two things. One is the magnitude of the magnetic moment of material. It is a vector with a fixed magnitude and direction that determines the torque seen by the magnet from an applied external magnetic field. Another characterization is the nature of the sign of the susceptibility, χ, of the material. This describes how a material responds when the external magnetic field is applied. Due to these different characterizations, magnetic materials divide into different types of magnetism; antiferromagnetism, paramagnetism, diamagnetism, ferromagnetism, and ferrimagnetism.

Ferromagnetism is the most obvious form of magnetism and has been known for several years. Without these materials compass, electromagnets, and generators could not be made and we literally would not be where we are today. Ferromagnets have a positive value of susceptibility and magnetic moments which align parallel with an externally applied field. It increases the total magnetism and maintains it even when the externally applied field is removed. When it crosses a specified critical temperature, a ferromagnet becomes paramagnetic, where the magnetic moments still align in the direction of the applied field but the alignment is much fragile than it is as compared below the critical temperature and the material no longer maintains its magnetism when the externally applied field is removed. Antiferromagnetic are like ferromagnets. The difference between the two is that their magnetic moments align antiparallel to the neighbouring moments.

This alignment occurs extemporaneously below a critical temperature known as the Neel temperature. The Neel temperature is named after Louis Neel, a scientist who discovered antiferromagnetism. He was awarded the Nobel Prize in 1970 in Physics for his work. Above the specified Neel temperature, the material becomes paramagnetic. Antiferromagnets are generally observed at low temperatures and are less frequent as compared to the other types of magnetic behaviours.

Geometry leads to magnetic properties

Antiferromagnetic materials usually align their magnetic moments antiparallel immediately when an external magnetic field is applied and the temperatures are below the critical temperature. The magnetization of an antiferromagnet always remains fixed or constant below the specific temperature called critical temperature and the material retains the antiparallel alignment when the externally applied magnetic field is removed. The magnetic moments are due to the spin part of the atomic valence electrons. If an external magnetic field is not applied to the material then the magnetic moments of all the orbiting electrons are all randomly oriented. When an external magnetic field is switched on in the material, the magnetic moments of the electrons start responding and align antiparallel to all the neighbouring moment. This is shown clearly in Figure 11.2.

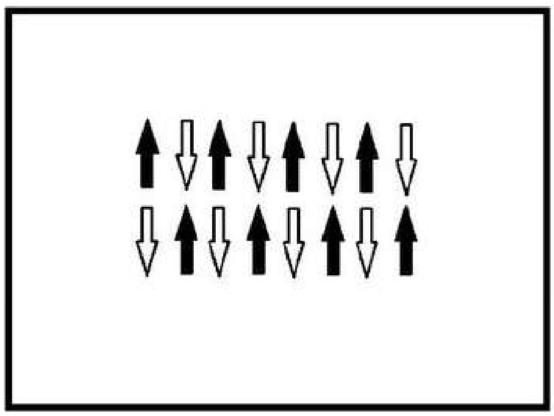


Fig. 11.2 *Antiferromagnetic Antiparallel Orientation of Magnetic Moments*

In a crystalline structure, one of the planes has a parallel spin alignment of ions with each other and the adjacent plane has the antiparallel spin alignment of ions, Figure 11.3. This generates two magnetic moments opposing each other in the sublattices and thus the resultant magnetic moment is zero.

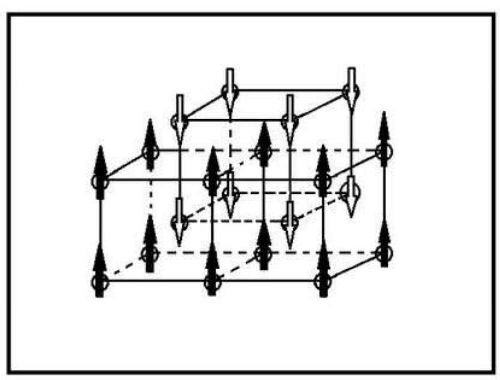


Fig. 11.3 *Schematic of the Antiferromagnetic Crystalline Structure of Sublattice with Opposing Magnetic Spins*

The antiparallel alignment is because of the superexchange of spin energy inside the material. One of the examples of the antiferromagnetic phenomenon is Manganese II oxide. MnO is an ionic compound that consists of linear chains of Mn2+ and O2- ions. The oxygen ion has a complete set of valence electrons in the p orbitals. These valence electrons are directly influencing the spin of the neighbouring Mn2+ ions. A diagrammatical presentation of the mechanism of superexchange is shown in Figure 11.4. This ionic compound possesses a degree of covalent bonding because it is energetically probable. Since both the ions Mn and O have full shells of electrons, Hence, hybridization happens due to the transfer of the O2- electrons to the open orbitals of the Mn2+ ions. The Mn2+ orbitals which already contain up-spin electrons accept one down-spin electron from the O2- p orbital leaving a single up-spin O2- electron. The O2- ion is then able to transfer its up-spin to the next Mn2+ ion in the chain which completes the bonds. The donation is possible only if the next Mn2+ ion has its d electrons available in the position of down-spin. According to Hund's Rule, all the unpaired electrons align with the parallel spins inside an orbital, so, all of the spins of Mn2+ electron must be flipped. This phenomenon is the superexchange. Hence, within the crystalline structure, the ions of Mn2+ are aligned with spins opposing each other.

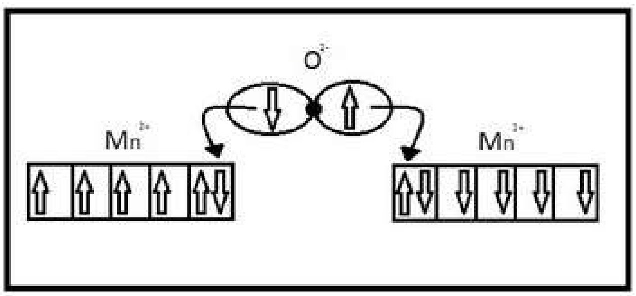


Fig. 11.4 *Schematic of Superexchange of MnO*

Temperature Dependence

The magnetic moment of antiferromagnetic material is depending on the temperature and their critical temperature is called as the Neel temperature, TN, at which a magnetic phase change occurs. In most of the cases, TN is below the room temperature but there are certain exceptions. When the temperature is above this temperature, the behavior of the material is paramagnetic with all the magnetic moments aligned with the direction of applied magnetic field. This enhances the overall magnetic field of the system. When the temperature is below the Neel temperature, the magnetic moments immediately align antiparallel and the total magnetization of the material is zero. This is due to the fact that the individual magnetic moments inside the sublattices cancel out. The susceptibility of the material also changes near the Neel temperature which is plotted in Figure 11.5. As the temperature is above TN, the susceptibility increases inversely and when the temperature is below this temperature, it decreases inversely.

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The dependence of paramagnetic materials on temperature can be determined by the Curie Law given by

$\chi = C / T$

Where the susceptibility is inversely related to the absolute temperature, T, and C is the Curie constant. The more specific and general Curie-Weiss Law gives

$\chi = C / T -$ ¸

Where Θ is another Curie constant in the units of temperature and it can be positive or negative depending on the material. Therefore, the susceptibility of the material is a function of temperature where an increase in temperature will decrease the material's responsiveness to the external applied magnetic field. The increase in the susceptibility for antiferromagnetic materials above the temperature TN leads to the negative value of Θ, see Figure 11.5. Hence, the Curie-Weiss Law for antiferromagnetic materials becomes

$\chi = C / T +$ ¸

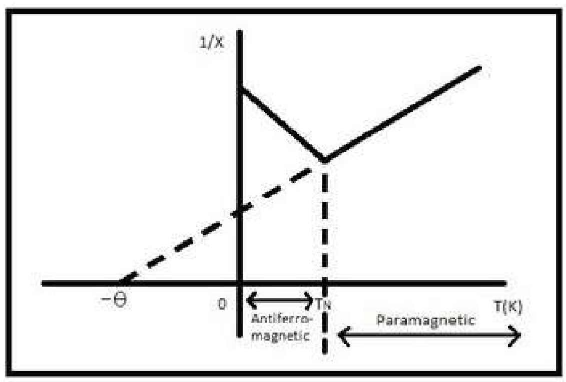


Fig. 11.5 *Temperature Dependence of Sntiferromagnets*

11.4 FERRIMAGNETISM AND FERRITES

Ferrimagnetism is a phenomenon in which the magnetic interaction between any two dipoles align anti-parallel to each other. But since the magnitude of dipoles are not equal, the cancellation of magnetic moments become incomplete resulting in a net magnetization in the material.

The magnetization of these materials is intermediate between ferromagnetic and antiferromagnetic materials.

General Properties of Ferrimagnetic Materials

1. Ferrimagnetic materials possess magnetic dipole moment due to the spin of the electrons.

2. The magnetic interaction between any two dipoles align themselves anti-parallel to each other. But, since the magnitude of moments are unequal, the cancellation of magnetic moments become incomplete resulting in a net magnetization in the materials.
3. A ferrimagnetic material is composed of more sets of different transition elements.
4. The susceptibility is very large and positive. It is given by $\chi = \frac{C}{T \pm \theta}$ when $T > T_N$. Beyond Neel temperature χ decreases as shown in Figure 11.6

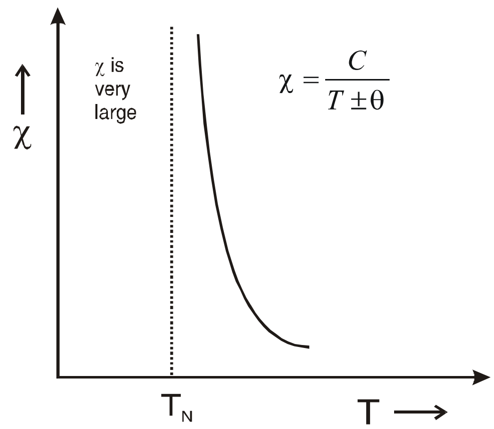


Fig. 11.6 *Variation of the Susceptibility with Temperature in Ferrimagnetic Material*

5. The most important ferrimagnetic materials are ferrites and rare earth garnets.
6. **Examples**: Nickel ferrite and ferrous ferrite.

FERRITES

Ferrites are compounds of iron oxides with oxides of other metals. The general chemical formula for a ferrite is $MOFe_2O_3$ or MFe_2O_4, where M is a divalent metal ion like Co, Ni, Mn, Mg, Zn, etc.

Many of them are magnetic materials and they are used to make permanent magnets, ferrite cores for transformers and in various other applications.

The structural, magnetic and elecrical properties of these ferrites are governed critically by their chemical composition. Ferrite can be prepared by conventional solid state method and numerous chemical methods such as, coprecipitation, solgel, aerogel and thermal decomposition process.

Ferrites could be obtained as soft magnetic ferrite and hard magnetic ferrites.

Soft magnetic ferrites have the components Magnese-Zinc, Lithium-Zinc, Nickel-Zinc and other types. Hard magnetic ferrites have the components iron, cobalt, barium and others.

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Properties

Ferrites are electrical insulators derived from iron oxides. But possess magnetic properties which are similar to those of ferromagnetic materials; such as, domain structure, hysteresis, etc. Not all ferrites are ferromagnetic but many are.

In general, ferrites are classified by (i) high magnetic permeability (ii) high remanent magnetic induction (iii) high value of saturation magnetization and (iv) high electrical resistance.

Note: • 1. **Soft magnetic ferrites** possess high value of magnetic permeability, saturation magnetization and remanent magnetization but low coercive force.
2. **Hard magnetic ferrites** possess high electrical resistance, coercive force and remanent magnetization .

Crystal Structure of Ferrites

Ferrites crystallise into the spinel structure which is named after the mineral, spinel ($MgAl_2O_4$).

The oxygen ions (O^{2-}) in a ferrite (MFe_2O_4) form a close packed structure. Each cubic cell contains eight formula unit. Thus there are, 32 O^{2-} ions, 16 Fe^{3+} ions and 8 M^{2+} ions in a unit cell. Thus there are, 24 (16+8) metallic ions or cations distributed amongst eight tetrahedral sites (also called A-sites, which has four nearest O^{2-} ions) and 16 octahedral sites (also called B-sites which has six nearest O^{2-} ions).

The distribution of metal ions (Fe^{3+} and M^{2+}) plays an important role in the magnetic behaviour of ferrite. In general, a distinction is made between spinel structures depending on the metallic ions that occupy A and B sites and the order in which the sites are occupied. The metal ions in tetrahedral and octahedral sites is shown in Figure 11.7.

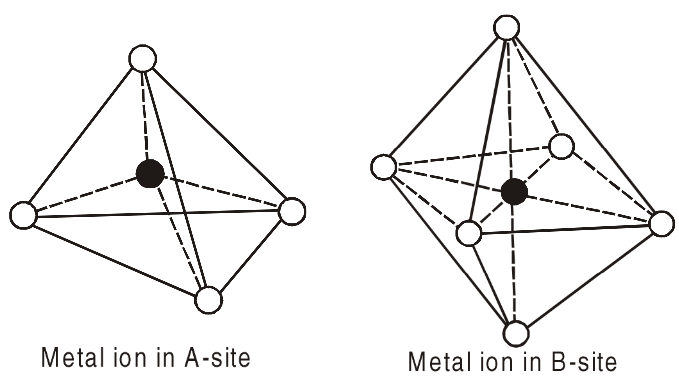


Fig. 11.7 *Metal Ions in Tetrahedral and Octahedral Sites*

1. Normal (Regular) Spinel Structure (Non Magnetic Spinel Ferrite)

In normal spinel structure of ferrites, eight divalent metal ions (M^{2+}) occupy tetrahedral or A-sites (has four nearest oxygen ions) and 16 trivalent metal ions (Fe^{3+}) occupy octahedral or B-sites (has six nearest O^{2-} ions). The arrangement

is shown in Figure 11.8. The usual notation for this structure is $M^{2+}[Fe_2^{3+}]O_4$. The [ ] bracket around Fe^{3+} ions denotes that they occupy octahedral sites.

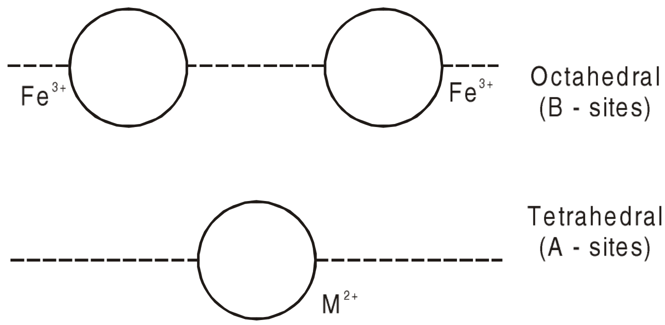


Fig. 11.8 *Normal (regular) spinel structure*

2. Inverse Spinel Structure (Ferrimagnetic Spinel Ferrite)

In the inverse spinel structure of ferrites, eight divalent metal ions (M^{2+}) occupy octahedral or B-sites and Fe^{3+} ions are distributed in equal numbers over tetrahedral or A-site and octahedral or B-sites. The usual notation for this structure is $Fe^{3+}[Fe^{3+}M^{2+}]O_4$. The ions within the [ ] occupy octahedral sites. This arrangement is shown in Figure 11.9.

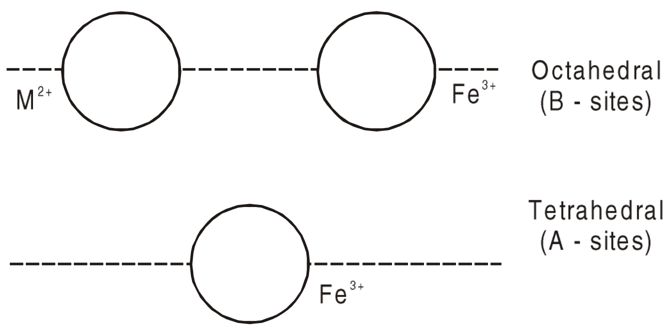


Fig. 11.9 *Inverse Spinel Structure*

Note: • Apart from spinel type crystal structure, ferrites also exists in garnet type with cubic crystal structure and magneto plembite type with hexagonal crystal structure.

Magnetization in a Ferrite Molecule

Since ferrites are ionic compound, the saturation magnetization may be calculated from the number of unpaired spins of the ions.

For example, in iron ferrite $[Fe^{2+}Fe_2^{3+}O_4]$ with arrangement $Fe^{3+}[Fe^{3+}Fe^{2+}]O_4$, the ions Fe^{2+} (ferrous) and Fe^{3+} (ferric) each has six 3d and two 4s electrons. Each ferrous ion has lost two 4s electrons (pair up) and the six 3d electrons remain to give four unpaired electrons (Figure 11.10). A ferric ion has lost the two 4s electrons and one 3d electron thus five unpaired electrons remain (Figure 11.10). Thus Fe^{2+} ion and Fe^{3+} ion have four and five unpaired spins. Therefore, the total dipole moment is $[4+(2\times 5)] = 14\ \mu_B$, where μ_B is

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the Bohr magneton. Here the dipole moment produced by one unpaired electron is taken as one Bohr magneton.

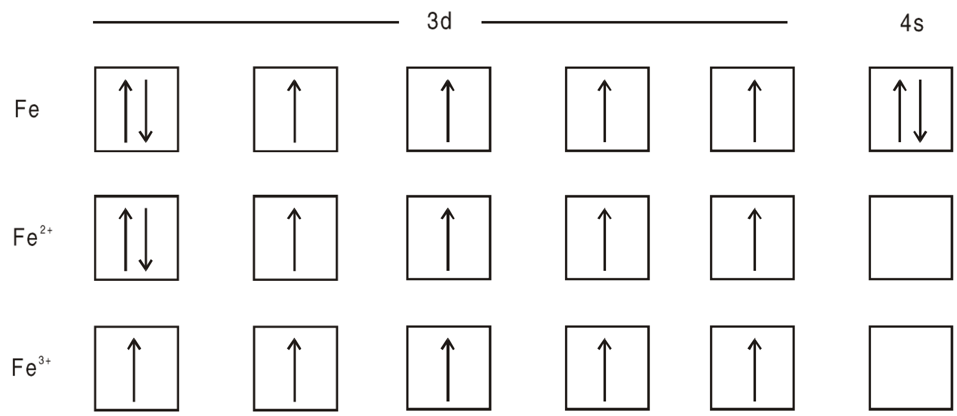


Fig. 11.10 *Unbalanced Magnetic Spins in Iron*

But from experiment, iron ferrite has only 4.08 μ_B. Thus it appears that, only Fe^{2+} ions contribute to magnetization. The iron ferrite (Fe_3O_4) has inverse spinel structure as shown in Figure 11.11.

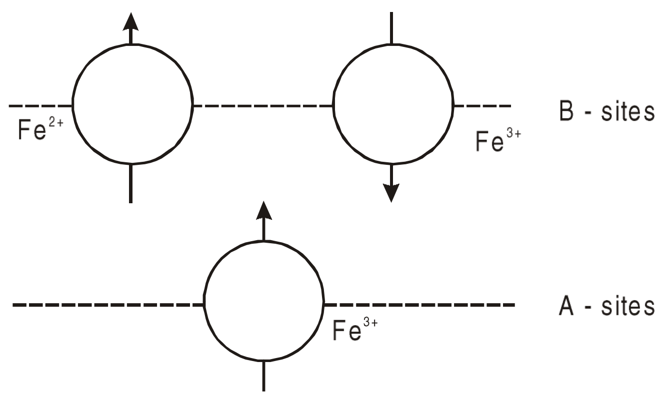


Fig. 11.11 *Ground State Spin Direction in Iron Ferrite (Fe_3O_4) with Inverse Spinel Structure*

Since Fe^{3+} ions magnetization cancel each other due to anti-parallel alignment, the net magnetic moment will be equal to 4 μ_B which is equal to the Bohr magneton of the divalent metal ions.

For all other ferrites such as Mg, Mn, Co which have inverse spinel structure, the ground state spin direction will be as shown in Figure 11.12

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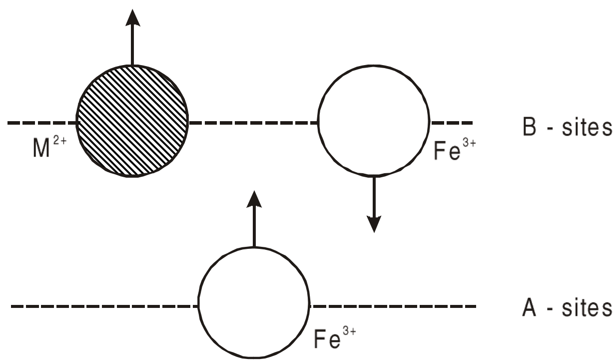


Fig. 11.12 *Ground State Spin Direction in $M^{2+}Fe_2O_4$ Ferrite with Inverse Spinel Structure*

In the examples given below, since Fe^{3+} ions spin magnetic moment cancel each other due to anti-parallel alignment, the net magnetic moment will be equal to the Bohr magneton of the respective divalent metal ions.

Examples:

Ferrite structure	A - site	B - site	Net magnetic moment
1. Fe_3O_4 Inverse spinel	Fe^{3+} ↓ $5\mu_B$	Fe^{3+} ↑ $5\mu_B$; Fe^{2+} ↑ $4\mu_B$	$4\mu_B$
2. $MnFe_2O_4$ Inverse spinel	Fe^{3+} ↓ $5\mu_B$	Fe^{3+} ↑ $5\mu_B$; Mn^{2+} ↑ $5\mu_B$	$5\mu_B$
3. $CdFe_2O_4$ Normal spinel	Cd^{2+} $0\mu_B$	Fe^{3+} ↑ $5\mu_B$; Fe^{3+} ↓ $5\mu_B$	$0\mu_B$
4. $ZnFe_2O_4$ Normal spinel	Zn^{2+} $0\mu_B$	Fe^{3+} ↑ $5\mu_B$; Fe^{3+} ↓ $5\mu_B$	$0\mu_B$

In examples three and four there is no magnetic moment in A-sites. Even though they are ferrites, they show no magnetization and hence antiferromagnetic materials.

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Note: • The magnetic moment of a ferrite material is found to be equal to the difference in the total moments of ions in A and B sites.

Applications of Ferrites

1. Soft magnetic ferrites are used in the production of cores for inductor coils used in telecommunications.
2. They are used in microwave applications such as isolator.
3. Ferrites are used in radio receivers to increase the sensitivity and selectivity of the receiver.
4. They are used to produce ultrasonic waves.
5. Ferrites are used in magnetic discs or tapes which store information.
6. Hard magnetic ferrites are used in the manufacturing of permanent magnets.
7. Ferrox cube is a soft ferrite magnetic material which has square hysteresis loop. These have high permeability and high resistivity. Because of these properties, they are used in switching circuits, matrix storage and in shift registers of computers.

   Example: Magnesium - magnese ferrite.

Check Your Progress

1. What do you understand by the antiferromagnetism?
2. Explain the general properties of antiferromagnetic materials.
3. Elaborate on the Neel's theory.
4. Define the term ferrimagnetism.
5. Illustrate the general properties of ferrimagnetic materials.
6. What do you mean by the ferrites?
7. State the general properties of ferrites.
8. Define the magnetization in a ferrite molecule.
9. Interpret the applications of ferrites.

11.5 ANSWERS TO CHECK YOUR PROGRESS QUESTIONS

1. Antiferromagnetism refers to a phenomenon in which the magnetic interaction between any two dipoles align themselves anti-parallel to each other. Since all the dipoles are of equal magnitude, the net magnetization is zero.

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2. Like ferromagnetic materials antiferromagnetic materials also possess dipole moment due to spin of the electron. These materials have a temperature dependent magnetism due to the disruption of the magnetic moment alignment.
3. In 1949 French physicist Louis Neel (1904-2000) discovered that when they are finely divided, ferromagnetic nanoparticles lose their hysteresis below a certain size; this phenomenon is known as superparamagnetism. The magnetization of these materials is subject to the applied field, which is highly non-linear.
4. Ferrimagnetism is a phenomenon in which the magnetic interaction between any two dipoles align anti-parallel to each other. But since the magnitude of dipoles are not equal, the cancellation of magnetic moments become incomplete resulting in a net magnetization in the material.
5. Ferrimagnetic materials possess magnetic dipole moment due to the spin of the electrons. A ferrimagnetic material is composed of more sets of different transition elements. The most important ferrimagnetic materials are ferrites and rare earth garnets.
6. Ferrites are compounds of iron oxides with oxides of other metals. The general chemical formula for a ferrite is $MOFe_2O_3$ or MFe_2O_4, where M is a divalent metal ion like Co, Ni, Mn, Mg, Zn, etc. Ferrites could be obtained as soft magnetic ferrite and hard magnetic ferrites.
7. Ferrites are electrical insulators derived from iron oxides. But possess magnetic properties which are similar to those of ferromagnetic materials; such as, domain structure, hysteresis, etc. Not all ferrites are ferromagnetic but many are.
8. Since ferrites are ionic compound, the saturation magnetization may be calculated from the number of unpaired spins of the ions.
9. They are used in microwave applications such as isolator. Ferrites are used in radio receivers to increase the sensitivity and selectivity of the receiver. They are used to produce ultrasonic waves. Ferrites are used in magnetic discs or tapes which store information.

11.6 SUMMARY

- Antiferromagnetism refers to a phenomenon in which the magnetic interaction between any two dipoles align themselves anti-parallel to each other. Since all the dipoles are of equal magnitude, the net magnetization is zero.
- Like ferromagnetic materials antiferromagnetic materials also possess dipole moment due to spin of the electron. These materials have a temperature dependent magnetism due to the disruption of the magnetic moment alignment.

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- The magnetic interaction between any two dipoles align themselves anti-parallel to each other. Since all the dipoles are equal in magnitude and due to anti-parallel alignment, the resultant magnetic effect is zero.
- In 1949 French physicist Louis Neel (1904-2000) discovered that when they are finely divided, ferromagnetic nanoparticles lose their hysteresis below a certain size; this phenomenon is known as superparamagnetism. The magnetization of these materials is subject to the applied field, which is highly non-linear.
- Ferrimagnetism is a phenomenon in which the magnetic interaction between any two dipoles align anti-parallel to each other. But since the magnitude of dipoles are not equal, the cancellation of magnetic moments become incomplete resulting in a net magnetization in the material.
- The magnetic interaction between any two dipoles align themselves antiparallel to each other. But, since the magnitude of moments are unequal, the cancellation of magnetic moments become incomplete resulting in a net magnetization in the materials.
- Ferrimagnetic materials possess magnetic dipole moment due to the spin of the electrons. A ferrimagnetic material is composed of more sets of different transition elements. The most important ferrimagnetic materials are ferrites and rare earth garnets.
- Ferrites are compounds of iron oxides with oxides of other metals. The general chemical formula for a ferrite is $MOFe_2O_3$ or MFe_2O_4, where M is a divalent metal ion like Co, Ni, Mn, Mg, Zn, etc. Ferrites could be obtained as soft magnetic ferrite and hard magnetic ferrites.
- The structural, magnetic and electrical properties of these ferrites are governed critically by their chemical composition. Ferrite can be prepared by conventional solid state method and numerous chemical methods such as, precipitation solgel, aerogel and thermal decomposition process.
- Since ferrites are ionic compound, the saturation magnetization may be calculated from the number of unpaired spins of the ions.
- Ferrites are used in radio receivers to increase the sensitivity and selectivity of the receiver. They are used to produce ultrasonic waves. Ferrites are used in magnetic discs or tapes which store information.

11.7 KEY WORDS

- **Antiferromagnetism:** Antiferromagnetism refers to a phenomenon in which the magnetic interaction between any two dipoles align themselves anti-parallel to each other. Since all the dipoles are of equal magnitude, the net magnetization is zero.

NOTES

- **Neel's theory:** In 1949 French physicist Louis Neel (1904-2000) discovered that when they are finely divided, ferromagnetic nanoparticles lose their hysteresis below a certain size; this phenomenon is known as superparamagnetism.
- **Ferrimagnetism:** Ferrimagnetism is a phenomenon in which the magnetic interaction between any two dipoles align anti-parallel to each other.
- **Ferrites:** Ferrites are compounds of iron oxides with oxides of other metals. The general chemical formula for a ferrite is $MOFe_2O_3$ or MFe_2O_4, where M is a divalent metal ion like Co, Ni, Mn, Mg, Zn, etc.

11.8 SELF ASSESSMENT QUESTIONS AND EXERCISES

Short-Answer Questions

1. Elaborate on the antiferromagnetism?
2. Define the general properties of antiferromagnetic materials.
3. Explain the Neel's theory.
4. What do you understand by the ferrimagnetism?
5. Interpret the general properties of ferrimagnetic materials.
6. What do you mean by the ferrites?
7. State the general properties of ferrites.
8. Explain the magnetization in a ferrite molecule.
9. Illustrate the applications of ferrites.

Long-Answer Questions

1. Discuss briefly the antiferromagnetism. Give appropriate examples.
2. Analyse the Neel's theory.
3. Explain the ferrimagnetism with the help of examples.
4. What are ferrites? Write the applications of ferrites.

11.9 FURTHER READINGS

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UNIT 12 MAGNETIC MATERIALS

NOTES

Structure

12.0 Introduction
12.1 Objectives
12.2 Spin Waves
12.3 Hard and Soft Magnetic Materials
12.4 Answers to Check Your Progress Questions
12.5 Summary
12.6 Key Words
12.7 Self Assessment Questions and Exercises
12.8 Further Readings

12.0 INTRODUCTION

The materials which are considered, explored, and used mainly for their magnetic properties, called magnetic materials. The magnetic property of a materials is largely determined by the magnetic dipole moment associated with the intrinsic angular momentum, or spin, of its electrons.

Magnetic materials are classified according to their bulk susceptibility. Ferromagnetism is responsible for most of the effects of magnetism encountered in everyday life, but there are actually several types of magnetism. Paramagnetic substances, such as aluminium and oxygen, are weakly attracted to an applied magnetic field; diamagnetic substances, such as copper and carbon, are weakly repelled; while antiferromagnetic materials, such as chromium and spin glasses, have a more complex relationship with a magnetic field. The force of a magnet on paramagnetic, diamagnetic, and antiferromagnetic materials is usually too weak to be felt and can be detected only by laboratory instruments, so in everyday life, these substances are often described as non-magnetic.

The magnetic state (or magnetic phase) of a material depends on temperature, pressure, and the applied magnetic field. A material may exhibit more than one form of magnetism as these variables change. Only magnetic dipoles have been observed, although some theories predict the existence of magnetic monopoles.

The magnetic properties of materials are mainly due to the magnetic moments of their atoms' orbiting electrons. The magnetic moments of the nuclei of atoms are typically thousands of times smaller than the electrons' magnetic moments, so they are negligible in the context of the magnetization of materials. Nuclear magnetic moments are nevertheless very important in other contexts, particularly in Nuclear Magnetic Resonance (NMR) and Magnetic Resonance Imaging (MRI).

In this unit, you will study about the spin waves, hard magnetic materials, and soft magnetic materials.

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12.1 OBJECTIVES

After going through this unit, you will be able to:

- Elucidate on the spin waves
- Define the hard magnetic materials
- Understand the soft magnetic materials

12.2 SPIN WAVES

A spin wave is a propagating disruption in the reference of a magnetic material. These low-lying collective excitations occur in magnetic lattices with continuous symmetry. From the equivalent quasi-particle point of view, spin waves are known as magnons, which are bosonic modes of the spin lattice that correspond roughly to the phonon excitations of the nuclear lattice. As temperature is increased, the thermal excitation of spin waves reduces a ferromagnet's spontaneous magnetization. The energies of spin waves are typically only μ_e V in keeping with typical Curie points at room temperature and below.

Spin waves are observed through four experimental methods: inelastic neutron scattering, inelastic light scattering (Brillouin scattering, Raman scattering and inelastic *X*-ray scattering), inelastic electron scattering (spin-resolved electron energy loss spectroscopy), and spin-wave resonance (ferromagnetic resonance).

The simplest way of understanding spin waves is to consider the Hamiltonian $\mathcal{H}$ for the Heisenberg ferromagnet:

$$\mathcal{H} = -\frac{1}{2}J\sum_{i,j}\mathbf{S}_i \cdot \mathbf{S}_j - g\mu_{\mathrm{B}}\sum_i \mathbf{H} \cdot \mathbf{S}_i$$

Where *J* is the exchange energy, the operators *S* represent the spins at Bravais lattice points, *g* is the Landé *g*-factor, μ_B is the Bohr magneton and **H** is the internal field which includes the external field plus any "Molecular" field. Note that in the classical continuum case and in 1 + 1 dimensions Heisenberg ferromagnet equation has the form,

$$\mathbf{S}_t = \mathbf{S} \times \mathbf{S}_{xx}.$$

In 1 + 1, 2 + 1 and 3 + 1 dimensions this equation admits several integrable and non-integrable extensions like the Landau-Lifshitz equation, the Ishimori equation, and so on. For a ferromagnet $J > 0$ and the ground state of the Hamiltonian $|0\rangle$ is that in which all spins are aligned parallel with the field **H**. That $|0\rangle$ is an

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Eigen state of $\mathcal{H}$ can be verified by rewriting it in terms of the spin-raising and spin-lowering operators given by:

$$S^{\pm} = S^{x} \pm iS^{y}$$

Resulting in,

$$\mathcal{H} = -\frac{1}{2}J\sum_{i,j} S_i^z S_j^z - g\mu_B H\sum_i S_i^z - \frac{1}{4}J\sum_{i,j}(S_i^+ S_j^- + S_i^- S_j^+)$$

Where z has been taken as the direction of the magnetic field. The spin-lowering operator S^- annihilates the state with minimum projection of spin along the z-axis, while the spin-raising operator S^+ annihilates the ground state with maximum spin projection along the z-axis.

12.3 HARD AND SOFT MAGNETIC MATERIALS

Both ferromagnetic and ferrimagnetic materials are classified either as soft or hard, based on the hysteresis characteristics.

The coercive field is the main parameter in distinguishing two types of magnetic materials namely, soft and hard.

Soft Magnetic Materials

Soft magnetic materials are characterised by a small hysteresis area and easy domain wall movement in the presence of an external magnetic field. These magnetic materials can be easily magnetised and demagnetised. But they cannot be permanently magnetised.

The nature of hysteresis curve for a soft magnetic material is shown in Figure 12.1.

Properties

Soft magnetic materials are characterised by the following properties.

1. Low coercivity
2. Low remanent magnetization
3. Low eddy current loss due to its higher resistivity
4. Low hysteresis energy loss (i.e., small hysteresis area)
5. High permeability
6. High susceptibility

The low coercivity and low remanent magnetization are due to the easy domain wall movement.

For easy domain wall movement, the material must be free from irregularities like strains, or impurities. Since the materials are free from irregularities, the magnetostatic energy is small.

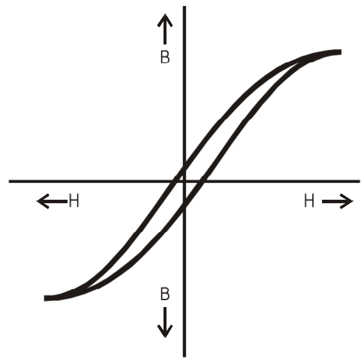


Fig. 12.1 *Hysteresis Curve for Soft Magnetic Material*

The soft magnetic materials have magnetic domains below Curie temperature. But during magnetization, the nature of domain wall motion is reversible.

As the domain wall motion is easy and also reversible, the coercive force assumes a small value and makes the hysteresis loop a narrow one. Because of this, the hysteresis loss becomes very small as shown in Figure 12.1. For the same reason, the materials can be easily magnetised and demagnetised.

For a magnet to be used in a.c. conditions, the magnet must have low hysteresis loss and low eddy current loss. In such a condition, a soft magnet is preferred.

In order to have the above mentioned properties to be possessed by a soft magnetic material the method of preparation plays a vital role.

The soft magnetic materials are prepared by heating the pure material to a temperature at which sufficient movement of the atoms is possible for them to settle down into an ordered lattice followed by slow cooling (annealing process).

Classification of Soft Magnetic Materials

Soft magnetic materials are classified into two categories.

1. Metallic soft magnetic materials.
2. Ceramic soft magnetic materials.

Examples

1. Iron and Silicon Alloys (Silicon Steel).
2. Iron - Nickel Alloys.
3. Iron - Cobalt Alloys.

4. Ferrite and Garnets.
5. Mu-Metal (Alloy of Ni, Cu, Cr and Fe).

Note: • **Garnets :** In general, garnets are ceramic oxides with general formula $M_3Fe_5O_{12}$, where M is trivalent metal ion with small ionic radius < 1 Å.

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Applications of Soft Magnetic Materials

1. Ferrites and garnets find wider application from audio to microwave frequency ranges.
2. Iron-nickel alloys are used for audio frequency applications.
3. Iron-silicon alloys are used for low frequency and high power applications.
4. Most of the soft magnetic materials are used as core materials in inductor coils and transformer.
5. Laminar sheets of soft magnetic materials are used in low frequency coils and transformers.
6. Both ferrites and garnets have very small eddy currents and hysteresis losses at microwave frequencies. Hence they are used in microwave devices such as gyrator, isolator, circulator, etc.
7. In digital computers and data processing circuits, soft magnetic materials with nearly rectangular hysteresis loop are used.
8. Based on the property of magnetostriction effect of soft magnetic materials, they are used for producing low frequency ultrasonic waves.
9. At radio frequencies, and in T.V, transformer ferrites are used.
10. Magnetic bubbles are used as memory storage device.

Hard Magnetic Materials

A hard magnetic material is characterised by a large hysteresis area and less mobile domain wall. These magnetic materials cannot be easily magnetised and demagnetised. But they can be permanently magnetised.

The nature of hysteresis curve for a hard magnetic material is shown in Figure 12.2.

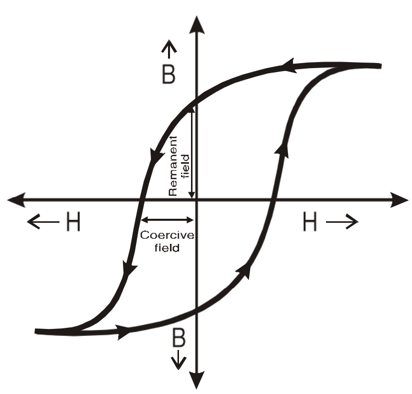


Fig. 12.2 *Hysteresis Curve for Hard Magnetic Material*

Properties

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Hard magnetic materials are characterised by the following properties.

1. High coercivity
2. High remanent magnetization
3. Relatively low permeability and susceptibility
4. High energy product (B_rH_c) or high power
5. High hysteresis energy loss due to large hysteresis area
6. More eddy current loss due to its smaller resistivity

The high coercivity and remanent magnetization are due to the less domain wall movement. In these materials, the domain wall movement is difficult and also irreversible due to the presence of impurities and crystal imperfections.

Because of the presence of impurities and crystal imperfections, the mechanical strain is more. Hence its magnetostatic energy is large.

These materials are prepared by heating the material to a required temperature and then suddenly cooling them (quenching process) by dipping in a cold liquid which sets up internal stresses. The mechanical strains are purposely introduced to make the magnetic materials hard.

Classification of Hard Magnetic Materials

Hard magnetic materials are classified into two categories.

1. Metallic hard magnetic materials
2. Ceramic hard magnetic materials.

Examples:

1. Platinum Cobalt Alloy
2. Tungsten Steel Alloy
3. Alnico Alloy (this is an Alloy of Al, Ni, Co, Cu and Fe)
4. Chromium Steel
5. Copper Nickel Iron Alloy (**Cunife**)
6. Copper Nickel Cobalt Alloy (**Cunico**)

Applicatioms of Hard Magnetic Materials

1. Hard magnetic materials are used for making permanent magnets.

2. Alloys of steel with tungsten and chromium are used in, magnetic separators, magnetic detectors, loudspeakers of audio system, microphones, flux meters, dc motors, etc.
3. Carbon steel is used in making magnets for toys and in certian types of measuring meters.

Check Your Progress

1. What do you mean by the spin waves?
2. Explain the soft magnetic materials.
3. Define the properties of soft magnetic materials.
4. Elaborate on the hard magnetic materials.
5. Illustrate the properties of hard magnetic materials.
6. What are the applications of hard magnetic materials?

12.4 ANSWERS TO CHECK YOUR PROGRESS QUESTIONS

1. A spin wave is a propagating disruption in the reference of a magnetic material. These low-lying collective excitations occur in magnetic lattices with continuous symmetry.
2. Soft magnetic materials are characterised by a small hysteresis area and easy domain wall movement in the presence of an external magnetic field. These magnetic materials can be easily magnetised and demagnetised. But they cannot be permanently magnetised.
3. Soft magnetic materials are characterised by the following properties:
   - o Low Coercivity,
   - o Low Remanent Magnetization
   - o Low Eddy Current Loss due to its Higher Resistivity
   - o High Permeability
   - o High Susceptibility
4. A hard magnetic material is characterised by a large hysteresis area and less mobile domain wall. These magnetic materials cannot be easily magnetised and demagnetised. But they can be permanently magnetised.

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5. Hard magnetic materials are characterised by the following properties:
   - o High Coercivity
   - o High Remanent Magnetization
   - o Relatively Low Permeability and Susceptibility
   - o High Hysteresis Energy Loss due to Large Hysteresis Area
   - o More Eddy Current Loss due to its Smaller Resistivity
6. Hard magnetic materials are used for making permanent magnets. Alloys of steel with tungsten and chromium are used in, magnetic separators, magnetic detectors, loudspeakers of audio system, microphones, flux meters, dc motors, etc.

12.5 SUMMARY

- A spin wave is a propagating disruption in the reference of a magnetic material. These low-lying collective excitations occur in magnetic lattices with continuous symmetry.
- As temperature is increased, the thermal excitation of spin waves reduces a ferromagnet's spontaneous magnetization. The energies of spin waves are typically only μ_e V in keeping with typical Curie points at room temperature and below.
- Spin waves are observed through four experimental methods: inelastic neutron scattering, inelastic light scattering (Brillouin scattering, Raman scattering and inelastic *X*-ray scattering), inelastic electron scattering (spin-resolved electron energy loss spectroscopy), and spin-wave resonance (ferromagnetic resonance).
- Soft magnetic materials are characterised by a small hysteresis area and easy domain wall movement in the presence of an external magnetic field. These magnetic materials can be easily magnetised and demagnetised. But they cannot be permanently magnetised.
- Hard magnetic materials are used for making permanent magnets. Alloys of steel with tungsten and chromium are used in, magnetic separators, magnetic detectors, loudspeakers of audio system, microphones, flux meters, dc motors, etc.

NOTES

12.6 KEY WORDS

- **Spin waves:** A spin wave is a propagating disruption in the reference of a magnetic material. These low-lying collective excitations occur in magnetic lattices with continuous symmetry.
- **Soft magnetic materials:** Soft magnetic materials are characterised by a small hysteresis area and easy domain wall movement in the presence of an external magnetic field.
- **Hard magnetic materials:** Hard magnetic materials are used for making permanent magnets. Alloys of steel with tungsten and chromium are used in, magnetic separators, magnetic detectors, loudspeakers of audio system, microphones, flux meters, dc motors, etc.

12.7 SELF ASSESSMENT QUESTIONS AND EXERCISES

Short-Answer Questions

1. Elaborate on the spin waves.
2. Define the soft magnetic materials.
3. Explain the properties of soft magnetic materials.
4. Illustrate the hard magnetic materials.
5. State the properties of hard magnetic materials.
6. Interpret the applications of hard magnetic materials?

Long-Answer Questions

1. Discuss briefly the spin waves. Give appropriate examples.
2. Analyse the soft magnetic materials with the help of examples.
3. Explain the hard magnetic materials with their properties.
4. Define the applications of soft and hard magnetic materials.

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NOTES

BLOCK - IV
SUPERCONDUCTIVITY

UNIT 13 SUPERCONDUCTIVITY-EXPERIMENTAL SURVEY

Structure

13.0 Introduction
13.1 Objectives
13.2 Superconductivity
13.3 Superconductor
13.4 Critical Temperature
13.5 Properties of Superconductors
13.6 Types of Superconductors
13.7 Answers to Check Your Progress Questions
13.8 Summary
13.9 Key Words
13.10 Self Assessment Questions and Exercises
13.11 Further Readings

13.0 INTRODUCTION

The superconductivity phenomenon was discovered in 1911 by Dutch physicist Heike Kamerlingh Onnes. Like ferromagnetism and atomic spectral lines, superconductivity is a phenomenon which can only be explained by quantum mechanics. Superconductivity is a set of physical properties observed in certain materials where electrical resistance vanishes and magnetic flux fields are expelled from the material. Any material exhibiting these properties is a superconductor.

Unlike an ordinary metallic conductor, whose resistance decreases gradually as its temperature is lowered even down to near absolute zero, a superconductor has a characteristic critical temperature below which the resistance drops abruptly to zero. An electric current through a loop of superconducting wire can persist indefinitely with no power source.

It is characterized by the Meissner effect, the complete ejection of magnetic field lines from the interior of the superconductor during its transitions into the superconducting state. The occurrence of the Meissner effect indicates that superconductivity cannot be understood simply as the idealization of perfect conductivity in classical physics.

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Experimental evidence points to a current lifetime of at least 100,000 years. Theoretical estimates for the lifetime of a persistent current can exceed the estimated lifetime of the universe, depending on the wire geometry and the temperature. It has been experimentally demonstrated that, as a consequence, when the magnetic field is increased beyond the critical field, the resulting phase transition leads to a decrease in the temperature of the superconducting material.

In this unit, you will study about the introduction of superconductivity-Experimental survey, the Meissner effect, isotope effect, type I and type II superconductors.

13.1 OBJECTIVES

After going through this unit, you will be able to:

- Understand the concept of superconductivity-experimental survey
- Analyse the Meissner effect
- Elaborate on the isotope effect
- Define the type I and type II superconductors

13.2 SUPERCONDUCTIVITY

Superconductivity *is a phenomenon in which certain metals, alloys and ceramics conduct electricity without resistance when, it is cooled below a certain temperature called the critical temperature.*

Superconductivity is a set of physical properties observed in certain materials where electrical resistance vanishes and magnetic flux fields are expelled from the material. Any material exhibiting these properties is a superconductor. Unlike an ordinary metallic conductor, whose resistance decreases gradually as its temperature is lowered even down to near absolute zero, a superconductor has a characteristic critical temperature below which the resistance drops abruptly to zero. An electric current through a loop of superconducting wire can persist indefinitely with no power source.

The superconductivity phenomenon was discovered in 1911 by Dutch physicist Heike Kamerlingh Onnes and it is still an exciting field of discovery and technological applications. This new state was first discovered in mercury when cooled below 4.2 K. Since then, a large number and wide variety of metals, alloys, binary and ternary chemical compounds have been found to show superconductivity at various temperatures.

Like ferromagnetism and atomic spectral lines, superconductivity is a phenomenon which can only be explained by quantum mechanics. It is characterized by the Meissner effect, the complete ejection of magnetic field lines from the interior

of the superconductor during its transitions into the superconducting state. The occurrence of the Meissner effect indicates that superconductivity cannot be understood simply as the idealization of perfect conductivity in classical physics.

In 1986, it was discovered that some cuprate-perovskite ceramic materials have a critical temperature above 90 K (“183 °C). Such a high transition temperature is theoretically impossible for a conventional superconductor, leading the materials to be termed high-temperature superconductors. The economically available coolant liquid nitrogen boils at 77 K, and thus the existence of superconductivity at higher temperatures than this facilitates many experiments and applications that are less practical at lower temperatures.

In the following sections fundamental terms and phenomena of superconductors, its properties, types and its applications are discussed in brief.

13.3 SUPERCONDUCTOR

A superconductor is a material that loses all its resistance (offers zero resistance) to the flow of electric current, when it is cooled below a certain temperature called the critical temperature or transition temperature T_c.

Examples : Mercury (Hg), Zinc (Zn), Vanadium (V), Tin (Sn) and Niobium (Nb).

A superconductor is a substance that conducts electricity without resistance when it becomes colder than a ‘Critical Temperature’. At this temperature, electrons can move freely through the material. Superconductors are different from ordinary conductors, even very good ones.

Ordinary conductors lose their resistance slowly as they get colder. In contrast, superconductors lose their resistance all at once. This is an example of a phase transition. High magnetic fields destroy superconductivity and restore the normal conducting state.

Normally, a magnet moving by a conductor produces currents in the conductor by electromagnetic induction. But a superconductor actually pushes out magnetic fields entirely by inducing surface currents. Instead of letting the magnetic field pass through, the superconductor acts like a magnet pointing the opposite way, which repels the real magnet. This is called the Meissner effect, and it can be demonstrated by levitating a superconductor over magnets or vice versa.

Physicists explain superconductivity by describing what happens when temperatures get cold. The thermal energy in a solid or liquid shakes the atoms so they randomly vibrate, but this gets less as the temperature drops. Electrons carry the same negative electric charge which makes them repel each other. At higher temperatures each electron behaves as if it were a free particle. There is also however a very weak attraction between electrons when they are in a solid or liquid. At rather large distances (many hundreds of nanometers apart) and low

temperatures (near absolute zero), the attractive effect and lack of thermal energy allows pairs of electrons to hang together. This is called a cooper pair and it is a quasiparticle, that is it acts as if it were a new kind of particle in its own right even though it is made up of two fundamental electrons. Many overlapping cooper pairs can exist in the same nanometer sized space. Since paired electrons constitute a boson the motions of all of the cooper pairs within a single superconductor synchronise and they function as if they are a single entity. Small disturbances, such as scattering of electrons are forbidden in this state and it moves as one showing no resistance to its motion. It is hence now a superconductor.

13.4 CRITICAL TEMPERATURE

The temperature at which a material's electrical resistivity drops to absolute zero is called the critical temperature or transition temperature T_c.

At and below T_c, the material is said to be in the superconducting state and above this temperature, the material is said to be in the normal state.

Figure 13.1 shows the variation of electrical resistivity of a normal metal silver (Ag) and a superconducting metal mercury (Hg) versus temperature.

From the Figure 13.1 it can be seen that, the electrical resistivity of normal metal decreases steadily as the temperature is decreased and reaches a low value at 0 K *called the residual resistivity* ρ_o. But in contrast, the electrical resistivity of mercury suddenly drops to zero at critical temperature T_c and is 4.2 K for Hg.

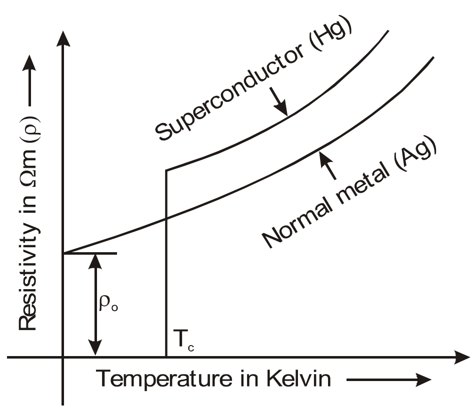


***Fig. 13.1** Electrical Resistivity Vs Temperature Plots for a Superconductor and a Normal Metal*

Note:
- Good electrical conductors such as silver (Ag), Gold (Au) and copper (Cu) are not good superconductors because, the resistivity of these conductors at low temperatures is limited to the low resistivity ρ_0 (residual resistivity) value due to scattering of electrons from crystal defects and impurities.
- Similarly, good superconducting materials like Zn and Pb are not good electrical conductors.

Below the critical temperature, not only does the superconductor suddenly achieve zero resistance, it exhibits a variety of several astonishing magnetic and electrical properties.

The T_c values for some selected metals, intermetallic and ceramic superconductors are given in the following Table 13.1.

Table 13.1 *T_C Values for Some Metals, Intermetallic and Ceramic Supercorductors*

Metals	T_c in K	Intermetallic compounds	T_c in K	Ceramic compounds	T_c in K
Tin (Sn)	3.72	NbTi	9.5	$Y_1\ Ba_2\ Cu_3\ O_{7-x}$	93
Mercury (Hg)	4.2	Nb_3Sn	21	Tl – Ba – Ca – Cu	125
Vanadium (V)	5.3	Nb_3Ge	23.2	HgBaCuO	133

13.5 PROPERTIES OF SUPERCONDUCTORS

Few important properties of superconductors are explained in brief in this section.

1. Electrical Resistance

The electrical resistance of a superconducting material is very low and is of the order of 10^{-7} Ωm.

2. Effect of Impurities

When impurities are added to superconducting elements, the superconducting property is not lost, but the T_c value is lowered.

3. Effect of Pressure and Stress

Certain materials are found to exhibit the superconductivity phenomena on increasing the pressure over them. For example, cesium is found to exhibit superconductivity phenomena at T_c = 1.5 K on applying a pressure of 110 Kbar.

In superconductors, the increase in stress results in increase of the T_c value.

4. Isotope Effects

The critical or transition temperature T_c value of a superconductor is found to vary with its isotopic mass. This variation in T_c with its isotopic mass is called the isotopic effect.

The relation between T_c and the isotopic mass is given by

$$T_c \propto^{al} \frac{1}{\sqrt{M}} \text{ where M is the isotopic mass.}$$

i.e., the transition temperature is inversely proportional to the square root of the isotopic mass of a single superconductor.

5. Magnetic Field Effect

If a sufficiently strong magnetic field is applied to a superconductor at any temperature below its critical temperature T_c, the superconductor is found to undergo a transition from the superconducting state to the normal state.

This minimum magnetic field required to destroy the superconducting state is called the ***critical magnetic field*** $\boldsymbol{H_c}$.

The critical magnetic field of a superconductor is a function of temperature. The variation of H_c with temperature is given by

$$H_c = H_o\left[1-\left(\frac{T}{T_c}\right)^2\right] \qquad ...(13.1)$$

where H_o is the critical field at T = 0 K. The critical field decreases with increasing temperature and, becoming zero at $T = T_c$.

Figure 13.2 shows the variation of critical field H_c as a function of temperature. The material is said to be in the superconducting state within the curve and is non superconducting (i.e., normal state) in the region outside the curve.

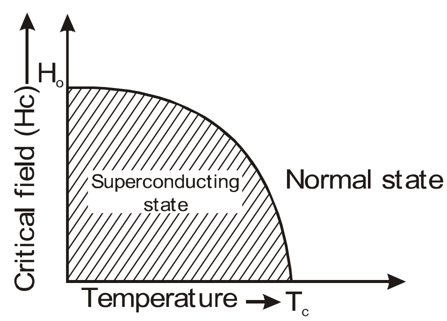


Fig. 13.2 *Dependence of H_c on T*

6. *Critical Current Density J_c and Critical Current I_c*

The critical current density is an another important characteristic feature of the superconducting state.

When the current density through a superconducting sample exceeds a critical value J_c, the superconducting state is found to disappear in the sample. This happens because, the current through the superconductor itself generates a magnetic field, and at a sufficiently high current density the magnetic field will start exceeding the critical magnetic field H_c thereby making the superconducting state to disappear in the material.

Hence, the critical current density can be defined as the maximum current that can be permitted in a superconducting material without destroying its superconductivity state. The critical current density is a

function of temperature, i.e., colder the temperature for a superconductor the more is the current it can carry.

For a thin long cylindrical superconducting wire of radius r the relation between critical current I_c and critical magnetic field H_c is given by

$$I_c = 2\ \pi r\ H_c$$

Similarly, the relation between critical current density J_c and critical current I_c is given by

$$J_c = \frac{I_c}{A}$$

where A is the superconducting specimen's cross-sectional area.

7. Persistent Current

When current is made to flow through a superconducting ring (say a loop of lead wire) which is at a temperature either equal to its T_c value or less than its T_c value, it was observed that the current was flowing through the material without any significant loss in its value.

This steady flow of current in a superconducting ring without any potential deriving it, is called the persistent current.

8. Meissner Effect (Diamagnetic Property)

*The complete expulsion of all the magnetic field by a superconducting material is called the **"Meissner Effect".***

When a superconducting material is placed in a magnetic field ($H > H_c$) at room temperature, the magnetic field is found to penetrate normally throughout the material, Figure 13.3(*a*).

However, if the temperature is lowered below T_c and with $H < H_c$ the material is found to reject all the magnetic field penetrating through it as shown in Figure 13.3(*b*).

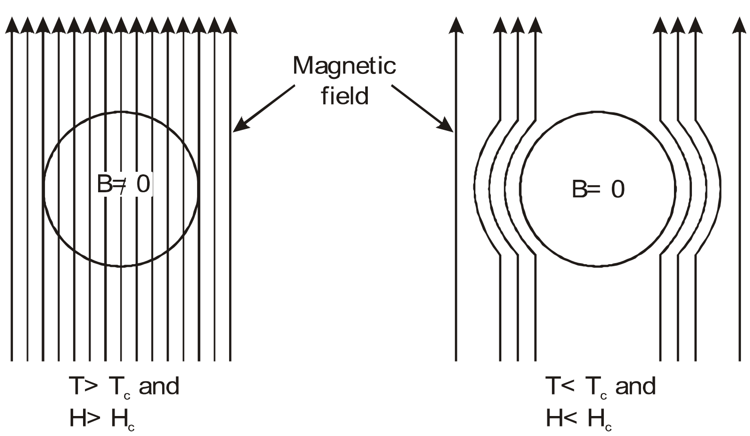


Fig. 13.3(a): *Normal State* ***Fig. 13.3(b):*** *Superconducting State*

NOTES

The above process occurs due to the development of surface current which inturn results in the development of magnetization M within the superconducting material. Hence, as the developed magnitation and the applied field are equal in magnitude but opposite in direction they cancel each other everywhere inside the material. Thus, below T_c a superconductor is a perfectly diamagnetic substance ($\chi_m = -1$).

The Meissner effect is a distinct characteristic of a superconductor from a normal perfect conductor. In addition, this effect is exhibited by the superconducting materials only when the applied field is less than the critical field H_c.

To prove $\chi_m = -1$ for Superconductors

We know that, for a magnetic material the magnetic induction or magnetic flux density B is given by

$$B = \mu_o (M + H) \qquad ...(13.2)$$

Where μ_o is the permeability of free space

M is the intensity of magnetisation

And, H is the applied magnetic field.

But, we know that for a superconductor B = 0

Therefore, Equation (13.2) can be written as

$$0 = \mu_o (M + H)$$

$$\because \quad \mu_o \neq 0$$

$$M + H = 0$$

or $$M = -H$$

or $$\frac{\mathbf{M}}{\mathbf{H}} = \mathbf{-1}$$

Hence, $\chi_m = -1$ *where* $\chi_m = \dfrac{M}{H}$ *is called the magnetic susceptibility.*

Thus this means that, for a superconductor the susceptibility is negative and maximum, i.e., a superconductor exhibits perfect diamagnetism.

Three Important Factors to Define a Superconducting State

In general, the superconducting state is defined by three important factors:

1. Critical Temperature T_c.
2. Critical Current Density J_c.
3. Critical Magnetic Field H_c.

Each of the above three parameters is very dependent on the other two properties. To sustain superconducting state in a material it is required to have both the current density and magnetic field, as well as the temperature, to remain below their critical values; and all of which depend on the material.

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The relationship between T_c, J_c and H_c is shown in the phase diagram Figure 13.4.

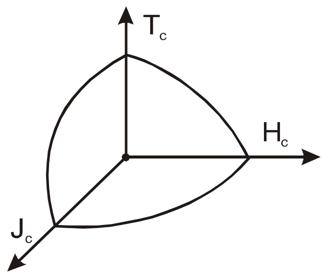


Fig. 13.4 *Critical Surface Phase Diagram*

The highest values for H_c and J_c occur at 0 K, while the highest value for T_c occurs when H and J are zero. Thus, the plot of all these three parameters represents a critical surface.

Within the surface the material is superconducting and outside the surface the material is said to be in the normal state.

Example 13.1

For mercury of mass number 202, the α value is 0.50 and T_c is 4.2 K. Find the transition temperature for the isotope of mercury of mass number 200.

Solution:

Given

Mass Number $M_1 = 202$

$\alpha = 0.5$

$T_{c1} = 4.2$ K

Mass Number $M_2 = 200$

$T_{c2} = ?$

We know, $M^\alpha\ T_{c1} = \text{Constant}$

Using this,

$$M_1^\alpha\ T_{c1} = M_2^\alpha\ T_{c2}$$

or

$$T_{c2} = \left(\frac{M_1}{M_2}\right)^\alpha T_{c1} = \left(\frac{202}{200}\right)^{0.5} \times 4.2 \qquad \left[\because \alpha = \frac{1}{2}\right]$$

$$= 1.004987 \times 4.2$$

$$\mathbf{T_{c2} = 4.2209\ K.}$$

Example 13.2

The critical temperature of Nb is 9.15 K. At zero kelvin the critical field is 0.196 T. Calculate the critical field at 6 K.

NOTES

Solution:

Given, $T_c = 9.15$ K; $T = 6$ K; $H_o = 0.196$ T; $H_c = ?$

$$H_c = H_o\left(1-\left(\frac{T}{T_c}\right)^2\right) = 0.196\left[\left(1-\left(\frac{6}{9.15}\right)^2\right)\right]$$

$$= 0.196\ [1 - 0.4299]$$

$$= 0.196\ [0.5701]$$

$$\therefore \quad \mathbf{H_c = 0.1117\ T.}$$

Example 13.3

The critical temperature for a metal with isotopic mass 199.5 is 4.185 K. Calculate the isotopic mass if the critical temperature falls to 4.133 K.

Solution:

Given, $M_1 = 199.5$; $T_{c1} = 4.185$ K; $T_{c2} = 4.133$ K; $M_2 = ?$

Formula

$$M_1^{\alpha}\ T_{c1} = M_2^{\alpha}\ T_{c2}$$

$$\therefore \quad M_2^{\alpha} = (199.5)^{\alpha}\ \frac{4.185}{4.133}$$

$$M_2^{0.5} = (199.5)^{0.5} \times 1.01258$$

$$\left[\because \alpha = \frac{1}{2}\right]$$

$$\sqrt{M_2} = \sqrt{199.5} \times 1.01258 = 14.124 \times 1.01258$$

$$M_2 = (14.301)^2$$

$$\therefore \quad \mathbf{M_2 = 204.55.}$$

Example 13.4

Calculate the critical current through a long thin superconducting wire of radius 0.5 mm. The critical magnetic field is 13.2 kA/m.

Solution:

Given, $H_c = 7.2 \times 10^3$ A/m; $r = 0.5 \times 10^{-3}$m; $I_c = ?$

Formula

$$I_c = 2\pi r\ H_c$$

$$= 2 \times 3.14 \times 0.5 \times 10^{-3} \times 7.2 \times 10^3$$

$$\therefore \quad \mathbf{I_c = 22.608\ A.}$$

Example 13.5

Superconducting Sn has a critical temperature of 3.7 K at zero magnetic field and a critical field of 0.0306 T at 0 K. Find the critical field at 2 K.

NOTES

Solution:

Given, $T_c = 3.7$ K; $H_o = 0.0306$ T; $H_c = ?$; T = 2 K

Formula

$$H_c = H_o \left[1 - \left(\frac{T}{T_c}\right)^2\right] = 0.0306 \left[1 - \left(\frac{2.0}{3.7}\right)^2\right]$$

$$= 0.0306\ (1 - 0.29218) = 0.0306 \times 0.70782$$

$$\therefore \quad \mathbf{H_c = 0.021659\ tesla.}$$

Example 13.6

Calculate the critical current for a superconducting wire of lead having a diameter of 1 mm at 4.2 K. Critical temperature for lead is 7.18 K and H_c (0) = 6.5×10^4 A/m.

Solution:

Given, $H_o = 6.5 \times 10^4$ A/m; $T_c = 7.18$ K; $r = 0.5 \times 10^{-3}$ m; T = 4.2 K; $I_c = ?$; $H_c = ?$

Formula

$$H_c = H_o \left[1 - \left(\frac{T}{T_c}\right)^2\right] = 6.5 \times 10^4 \left[1 - \left(\frac{4.2}{7.18}\right)^2\right]$$

$$= 6.5 \times 10^4\ (1 - 0.34217) = 6.5 \times 10^4 \times 0.65783$$

$$\therefore \quad \mathbf{H_c = 42.758\ kA/m.}$$

$$I_c = 2\pi r\, H_c = 2 \times 3.14 \times 0.5 \times 10^{-3} \times 42.758 \times 10^3$$

$$\therefore \quad \mathbf{I_c = 134.26\ A.}$$

Example 13.7

The critical field for vanadium is 10^5 Am^{-1} at 8.58 K and 2×10^5 Am^{-1} at 0 K. Determine the T_c value.

Solution:

Given, $H_c = 10^5$ Am^{-1}; $H_o = 2 \times 10^5$ Am^{-1}; T = 8.58 K; $T_c = ?$

Formula

$$H_c = H_o \left[1 - \left(\frac{T}{T_c}\right)^2\right]$$

$$\therefore \quad \left(\frac{H_c}{H_o}\right) = 1 - \left(\frac{T}{T_c}\right)^2$$

$$\left(\frac{T}{T_c}\right)^2 = 1 - \left(\frac{H_c}{H_o}\right)$$

NOTES

$$\therefore \quad T_c = \frac{T}{\sqrt{1-\left(\frac{H_c}{H_o}\right)}} = \frac{8.58}{\sqrt{1-\frac{10^5}{2\times10^5}}} = \frac{8.58}{\sqrt{1-0.5}} = \frac{8.58}{\sqrt{0.5}} = \frac{8.58}{0.7071}$$

$$\therefore \quad \mathbf{T_c = 12.133\ K.}$$

13.6 TYPES OF SUPERCONDUCTORS

Based on the behaviour of superconducting materials in an applied magnetic field, the superconductors are classified into type I and II superconductors.

Type I Superconductors

Type I superconductors exhibit complete Meissner effect, i.e., they are completely diamagnetic. The magnetization curve for type I superconductor is shown in Figure 13.5(*a*). The values of H_c for type I superconducting materials are always too low.

The magnetization curve shows that, the transition at H_c is reversible; which means that, if the magnetic field is reduced below H_c, the material again acquires superconducting property and the field is expelled.

Type I superconductors are also called as ***soft superconductors*** because of their tendency to allow the field penetration even for a lower applied field. Many pure elements, alloys and some compound superconductors exhibit type I behaviour.

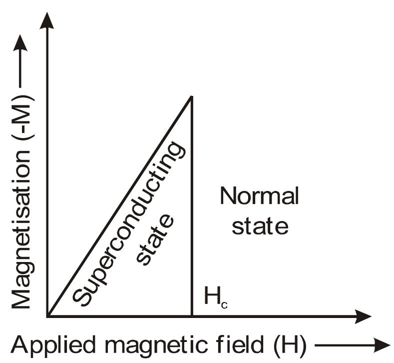


Fig. 13.5(a) *Type I Superconductor*

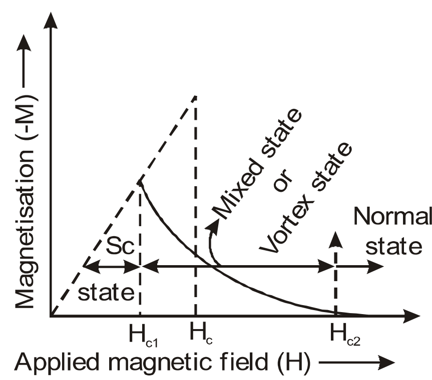


Fig. 13.5(b) *Type II Superconductor*

Type II Superconductors

Type II superconductors behave differently in an increasing field as shown in Figure 13.5(*b*). For an applied field below H_{c1}, the material is perfectly diamagnetic and hence the field is completely excluded. *H_{c1}, is called as lower*

NOTES

critical field. At H_{c1}, the field starts to thread the specimen and this penetration increases until H_{c2} is reached at which, the magnetization vanishes and the specimen becomes normal. *H_{c2} is called the upper critical field.*

In the region between H_{c1} and H_{c2} the material is in the mixed state or vortex state. The value of H_{c2} for type II may be 100 times more or even higher than that of type I superconducting material. As H_{c2} and T_c of type II superconducting materials are higher than that of type I superconductors, the type II superconducting materials are most widely used in all engineering applications.

Type I superconducting materials are also called as ***hard superconductors*** because of relatively large magnetic field requirement to bring them back to their normal state.

Table 13.2 *Examples of Type I and Type II Superconductors with their H_c Values*

Type I	Type II		
Material	H_c in tesla	Material	H_c in tesla
T*a*	0.083	$Y_1 Ba_2 Cu_3 O_7$	300
Pb	0.08	$Ba_{2-x} B_x Cu O_4$	150
Hg	0.014	Nb_3Sn	24.5
Sn	0.030	$Nb_3 Ge$	38

Examples for type I and type II superconducting materials with their H_c values are listed in Table 13.2.

Comparison between Type I and Type II Superconductors

Type I Superconductor	Type II Superconductor
1. These superconductors are called as soft superconductors.	1. These superconductors are called as hard superconductors.
2. Only one critical field exists for these superconductors. for these superconductors.	2. Two critical fields H_{c1} (lower critical field) and H_{c2} (upper critical field) exists.
3. The critical field value is very low.	3. The critical field value is very very high.
4. These superconductors exhibit perfect and complete Meissner effect.	4. These do not exhibit a perfect and complete Meissner effect.
5. These materials have limited technical applications because of very lower field strength value.	5. These materials have wider technological applications because of very higher field strength value.
Examples: Pb, Hg, Zn etc.	***Examples:*** Nb_3Ge, Nb_3Si, $Y_1Ba_2Cu_3O_7$ etc.

NOTES

Check Your Progress

1. Define the term superconductivity.
2. Elaborate on the superconductors.
3. Illustrate the critical temperature.
4. State the effect of impurities on superconductors.
5. What do you understand by the isotopic effect?
6. Explain the persistent current in superconductors.
7. Interpret the Meissner effect.
8. Define the three important factors to describe a superconducting state.
9. State the type I superconductors.
10. Explain the type II superconductors.

13.7 ANSWERS TO CHECK YOUR PROGRESS QUESTIONS

1. Superconductivity is a phenomenon in which certain metals, alloys and ceramics conduct electricity without resistance when, it is cooled below a certain temperature called the critical temperature.
2. A superconductor is a material that loses all its resistance (offers zero resistance) to the flow of electric current, when it is cooled below a certain temperature called the critical temperature or transition temperature T_c.
3. The temperature at which a material's electrical resistivity drops to absolute zero is called the critical temperature or transition temperature T_c.
4. When impurities are added to superconducting elements, the superconducting property is not lost, but the T_c value is lowered.
5. The critical or transition temperature T_c value of a superconductor is found to vary with its isotopic mass. This variation in T_c with its isotopic mass is called the isotopic effect.
6. The steady flow of current in a superconducting ring without any potential deriving it, is called the persistent current.
7. The complete expulsion of all the magnetic field by a superconducting material is called the "Meissner Effect". The Meissner effect is a distinct characteristic of a superconductor from a normal perfect conductor. In addition, this effect is exhibited by the superconducting materials only when the applied field is less than the critical field H_c.

8. In general, the superconducting state is defined by three important factors:
   - o Critical Temperature T_c
   - o Critical Current Density J_c
   - o Critical Magnetic Field H_c
9. Type I superconductors exhibit complete Meissner effect, i.e., they are completely diamagnetic. Type I superconductors are also called as soft superconductors because of their tendency to allow the field penetration even for a lower applied field. The values of H_c for type I superconducting materials are always too low.
10. Type II superconductors behave differently in an increasing field. For an applied field below H_{c1}, the material is perfectly diamagnetic and hence the field is completely excluded. H_{c1}, is called as lower critical field. Type II superconducting materials are also called as hard superconductors.

13.8 SUMMARY

- Superconductivity is a phenomenon in which certain metals, alloys and ceramics conduct electricity without resistance when, it is cooled below a certain temperature called the critical temperature.
- Superconductivity is a set of physical properties observed in certain materials where electrical resistance vanishes and magnetic flux fields are expelled from the material. Any material exhibiting these properties is a superconductor.
- Unlike an ordinary metallic conductor, whose resistance decreases gradually as its temperature is lowered even down to near absolute zero, a superconductor has a characteristic critical temperature below which the resistance drops abruptly to zero. An electric current through a loop of superconducting wire can persist indefinitely with no power source.
- The superconductivity phenomenon was discovered in 1911 by Dutch physicist Heike Kamerlingh Onnes and it is still an exciting field of discovery and technological applications. This new state was first discovered in mercury when cooled below 4.2 K. Since then, a large number and wide variety of metals, alloys, binary and ternary chemical compounds have been found to show superconductivity at various temperatures.
- A superconductor is a material that loses all its resistance (offers zero resistance) to the flow of electric current, when it is cooled below a certain temperature called the critical temperature or transition temperature T_c.
- The temperature at which a material's electrical resistivity drops to absolute zero is called the critical temperature or transition temperature T_c.

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- A superconductor is a substance that conducts electricity without resistance when it becomes colder than a 'Critical Temperature'. At this temperature, electrons can move freely through the material.
- Ordinary conductors lose their resistance slowly as they get colder. In contrast, superconductors lose their resistance all at once. This is an example of a phase transition. High magnetic fields destroy superconductivity and restore the normal conducting state.
- The electrical resistance of a superconducting material is very low and is of the order of 10^{-7} Ωm.
- When impurities are added to superconducting elements, the superconducting property is not lost, but the T_c value is lowered.
- Certain materials are found to exhibit the superconductivity phenomena on increasing the pressure over them. In superconductors, the increase in stress results in increase of the T_c value.
- The critical or transition temperature T_c value of a superconductor is found to vary with its isotopic mass. This variation in T_c with its isotopic mass is called the isotopic effect.
- The minimum magnetic field required to destroy the superconducting state is called the critical magnetic field H_c.
- The steady flow of current in a superconducting ring without any potential deriving it, is called the persistent current.
- The complete expulsion of all the magnetic field by a superconducting material is called the "Meissner Effect". The Meissner effect is a distinct characteristic of a superconductor from a normal perfect conductor.
- In addition, Meissner effect is exhibited by the superconducting materials only when the applied field is less than the critical field H_c.
- Type I superconductors exhibit complete Meissner effect, i.e., they are completely diamagnetic. Type I superconductors are also called as soft superconductors.
- Type II superconductors behave differently in an increasing field. Type II superconducting materials are also called as hard superconductors.

13.9 KEY WORDS

- **Superconductivity:** Superconductivity is a phenomenon in which certain metals, alloys and ceramics conduct electricity without resistance when, it is cooled below a certain temperature called the critical temperature.

- **Superconductor:** A superconductor is a material that loses all its resistance (offers zero resistance) to the flow of electric current, when it is cooled below a certain temperature called the critical temperature or transition temperature T_c.
- **Meissner effect:** The Meissner effect is a distinct characteristic of a superconductor from a normal perfect conductor.
- **Type I superconductors:** Type I superconductors exhibit complete Meissner effect, i.e., they are completely diamagnetic. Type I superconductors are also called as soft superconductors.
- **Type II superconductors:** Type II superconductors behave differently in an increasing field. Type II superconducting materials are also called as hard superconductors.

13.10 SELF ASSESSMENT QUESTIONS AND EXERCISES

Short-Answer Questions

1. Explain the term superconductivity.
2. Define superconductors.
3. Elaborate on the critical temperature.
4. Illustrate the effect of impurities on superconductors.
5. What do you mean by the isotopic effect?
6. Interpret the persistent current in superconductors.
7. Explain the Meissner effect.
8. Describe the three important factors to define a superconducting state.
9. Define the type I superconductors.
10. State the type II superconductors.

Long-Answer Questions

1. Briefly discuss about the superconductivity-experimental survey giving examples.
2. Explain the critical temperature with the help of examples.
3. Discuss briefly the properties of superconductors.
4. Analyse the Meissner effect.
5. Describe the types of superconductors giving appropriate examples.
6. Give a detailed comparison between the type I and type II superconductors.

NOTES

13.11 FURTHER READINGS

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UNIT 14 SUPERCONDUCTIVITY - THEORETICAL SURVEY

NOTES

Structure

14.0 Introduction
14.1 Objectives
14.2 London Equations
14.3 Coherence Length
14.4 Bcs Theory and Cooper Pair
14.5 Normal Tunnelling
14.6 High Temperature Superconductors
14.7 Answers to Check Your Progress Questions
14.8 Summary
14.9 Key Words
14.10 Self Assessment Questions and Exercises
14.11 Further Readings

14.0 INTRODUCTION

The superconductivity was discovered in 1911 by Dutch physicist Heike Kamerlingh Onnes. Superconductivity is a set of physical properties observed in certain materials where electrical resistance disappears and magnetic flux fields are expelled from the material. Any material exhibiting these properties is a superconductor.

Unlike an ordinary metallic conductor, whose resistance decreases gradually as its temperature is lowered even down to near absolute zero, a superconductor has a characteristic critical temperature below which the resistance drops abruptly to zero. An electric current through a loop of superconducting wire can persist indefinitely with no power source.

Like ferromagnetism and atomic spectral lines, superconductivity is a phenomenon which can only be explained by quantum mechanics. It is characterized by the Meissner effect, the complete ejection of magnetic field lines from the interior of the superconductor during its transitions into the superconducting state. The occurrence of the Meissner effect indicates that superconductivity cannot be understood simply as the idealization of perfect conductivity in classical physics.

Superconductors are used to build Josephson junctions which are the building blocks of SQUIDs (Superconducting Quantum Interference Devices), the most sensitive magnetometers known. SQUIDs are used in scanning SQUID microscopes and magnetoencephalography. Series of Josephson devices are used to realize the SI volt. Depending on the particular mode of operation, a superconductor–insulator–superconductor Josephson junction can be used as a photon detector or as a mixer. The large resistance change at the transition from

the normal- to the superconducting state is used to build thermometers in cryogenic micro-calorimeter photon detectors. The same effect is used in ultrasensitive bolometers made from superconducting materials.

In this unit, you will study about the London equations, coherence length, the BCS Theory, the Cooper pair, normal tunnelling, the Josephson effect, and high temperature superconductors.

14.1 OBJECTIVES

After going through this unit, you will be able to:

- Interpret the London equations
- Explain the coherence length
- Understand the BCS Theory
- Elaborate on the Cooper pair
- Define normal tunnelling
- Comprehend the Josephson effect
- Analyse the high temperature superconductors

14.2 LONDON EQUATIONS

In the Meissner effect, it is already discussed that one of the conditions of the superconducting state is that Magnetic flux density (B) = 0 inside the superconductors. This means that the magnetic flux cannot penetrate inside the superconductor. But experimentally it is not true. The magnetic flux does not suddenly goes to zero inside the surface. H. London and F. London has explained the phenomenon of flux penetration inside the superconductors.

This is already shown that the Meissner effect implies that the value of magnetic susceptibility $\chi = —1/4\Pi$ in CGS unit system in the superconducting state or, in SI, $\chi = -1$. Is it possible to modify a constitutive equation of electrodynamics (such as Ohm's law) by some method to get the Meissner effect? The modification in the Maxwell equations in not required. In the normal state of a metal electrical conduction is described by Ohm's law which is given by j = a-E. Now, we need to do the modification in this to describe conduction and the Meissner effect in the superconducting state. Let us first make a postulate and then see what happens next.

We put a postulate that when the current density is superconducting it is directly proportional to the vector potential A of the local magnetic field, where B = curl A. The gauge of A will be identified. In CGS units the constant of proportionality can be written as $—c/4\Pi\lambda_L^{\ 2}$ for reasons that will clear later.

Here c is the speed of light and λ_L is a constant with the dimensions of length.

The theoretical model that was first conceived for superconductivity was completely classical: it is summarized by London equations. It was put forward by the brothers Fritz and Heinz London in 1935, shortly after the discovery that magnetic fields are expelled from superconductors. A major triumph of the equations of this theory is their ability to explain the Meissner effect, wherein a material exponentially expels all internal magnetic fields as it crosses the superconducting threshold. By using the London equation, one can obtain the dependence of the magnetic field inside the superconductor on the distance to the surface.

The two constitutive equations for a superconductor by London are:

$$\frac{\partial \mathbf{j}}{\partial t} = \frac{ne^2}{m}\mathbf{E}, \qquad \nabla \times \mathbf{j} = -\frac{ne^2}{m}\mathbf{B}.$$

The first equation follows from Newton's second law for superconducting electrons.

Magnetic Levitation (Maglev)

Magnetic levitation or maglev is the process by which an object is suspended above another object with no other support but magnetic fields.

We know that, a diamagnetic substance repels a magnetic field. Thus, the perfect diamagnetic property of superconductors make them suitable for achieving friction less motion in motors and bearing.

The phenomena of magnetic levitation is based on Meissner effect.

How to Achieve Magnetic Levitation ?

The magnetic levitation is brought about by enormous repulsion between two highly powerful magnetic fields.

If a small magnet is brought near a superconductor it will be repelled. This repulsion takes place due to the induced currents in the superconductor which is being generated by the magnetic field of the magnet. Because of zero resistance property of the superconductor this current persists and thus, the field due to this induced current repels the field due to the magnet. As a result, the magnet floats freely (i.e., levitated) above the superconductor.

Thus, the levitation of the magnet or maglev demonstrates two critical properties of superconductors: (i) zero resistance and (ii) Meissner effect.

Applications

Magnetically levitated vechiles are called maglev vehicles. The utility of such levitation in vechiles is that, in the absence of contact between the moving and stationary systems, the friction is eliminated. With such an arrangement great speeds could be achieved with very low energy consumption.

NOTES

1. Maglev Train

The levitation is based on two techniques: (i) ElectroMagnetic Suspension (EMS) and (ii) ElectroDynamic Suspension (EDS).

In attractive EMS the electromagnets installed on the train bogies attract the iron rails (guideways). The vechile magnets wrap around the iron guideways and the attractive upward force lifts the train.

In EDS levitation is achived by creating a repulsive force between the train and guideways.

The basic idea of maglev train is to levitate it with magnetic fields so that there is no physical contact between the train and the rails (guideways). Consequently the maglev train can travel at very high speed. These trains travel at a speed of about 500 km/h.

2. A similar magnetic propulsion system is being used to launch the satellite into orbits directly from earth without the use of rockets.

Josephson Effect and its Application

Josephson Junction: *Two superconductors separated by a very thin strip of an insulator Figure 14.1 forms a Josephson junction.*

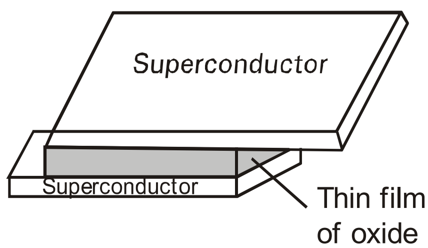


Fig. 14.1 *Josephson Junction*

Josephson Effect

The wave nature of moving particles makes the electrons to tunnel through the barrier (insulator), i.e., the electrons can tunnel from one superconductor to the other. As a consequence of the tunneling of electrons (cooper pairs) across the insulator, there is a net current across the junction. This is called as ***d.c. Josephson effect.*** The current flows even in the absence of a potential difference.

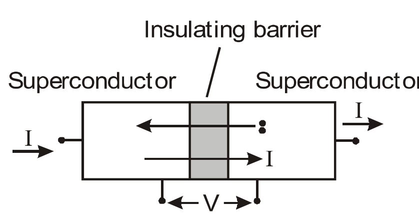


Fig. 14.2 *Josephson Junction with an Applied External Voltage (V)*

The magnitude of the current depends on, the thickness of the insulator, the material nature and on the temperature.

On the other hand, when a potential difference V is applied between the two sides of the junction Figure 14.2, there will be an oscillation of the tunneling current with angular frequency $\nu = \frac{2eV}{h}$. This is called the ***a.c. Josephson effect.*** Thus, according to a.c. Josephson effect, the junction generates an a.c. current at a frequency of $\frac{2eV}{h}$ Hz per volt.

Note: Cooper pair is a bound pair of electrons formed by the interaction between the electrons with opposite momenta and spin in a phonon field.

Application of Josephson Junction

Josephson junctions are used in sensitive magnetometers called SQUID-Superconducting Quantum Interference Device.

A SQUID is formed by connecting two Josephson junctions in parallel, Figure 14.3.

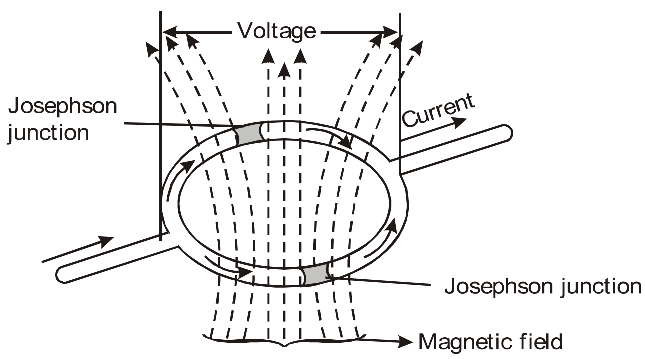


Fig. 14.3 *SQUID*

When current is passed into this arrangement, the current splits flowing across the two opposite arc. The current through the circuit will have a periodicity which is very sensitive to the magnetic flux passing normally through the closed circuit. As a result, extremely small magnetic flux can be detected with this device.

This device can also be used to detect voltages as small as 10^{-15} V.

Magnetic field changes as small as 10^{-21}T can be detected.

Weak magnetic fields produced by biological currents such as those in the brain can also be detected using SQUID's.

SQUID detectors are used to measure the levels of iron in liver, so that iron built up can be treated before much harm is done to the body.

NOTES

Other Applications of Superconductors

1. Superconductors can be used to transmit electrical power over very long distances, without any power loss or any voltage drop.
2. Superconducting generators has the benefit of small size and low energy consumption than the conventional generators.
3. Superconducting coils are used in N.M.R (Nuclear Magnetic Resonance) imaging equipments which are used in hospitals, for scanning the whole body to diagnose medical problems.
4. Very strong magnetic fields can be generated with coils made of high – T_c superconducting materials.
5. Superconductors can act as relay or switching system in a computer. They can also be used as a memory or storage element in computers.

   Cryotron : It is a relay or switch made of superconductors whose size can be made very small. In addition, these switches consume a very little current.

   The cryotron consists of two superconducting materials A and B. Let the material A be inside the coil of wire B as shown in Figure 14.4.

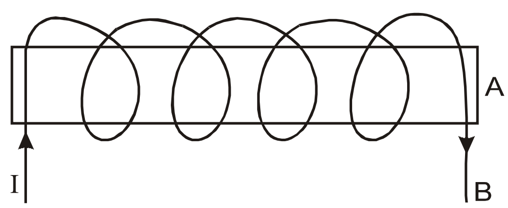
   

   Fig. 14.4 *Cryotron*

   Let the critical field of the material A be H_{cA} and that of B be H_{cB} respectively and also, let $H_{cA} < H_{cB}$. If a current I is passed through the material B, the current induces a magnetic field H. If this induced field H happens to be greater than H_{cA} then the superconducting property of the material A gets destroyed.

   Hence, the resistivity increases and the contact is broken. Thus, the current in A can be controlled by the current in B and hence, this system can act as a relay or switch element.
6. Very fast and accurate computers can be constructed using superconductors and the power consumption is also very low.
7. Ore separation can be done efficiently using superconducting magnets.

Example 14.8

A voltage of 5.9 μV is applied across a Josephson junction. What is the frequency of the radiation emitted by the junction?

Solution:

Given, $V = 5.9 \times 10^{-6}$ V; $\nu = ?$

Formula $\nu = \frac{2eV}{h} = \frac{2 \times 1.6 \times 10^{-19} \times 5.9 \times 10^{-6}}{6.62 \times 10^{-34}}$

$\nu = 2.851 \times 10^9$ **Hz.**

14.3 COHERENCE LENGTH

In condensed matter physics coherence length is the propagation distance over which a coherent wave (e.g., an electromagnetic wave) maintains a specified degree of coherence. Wave interference is strong when the paths taken by all of the interfering waves differ by less than the coherence length. A wave with a longer coherence length is closer to a perfect sinusoidal wave. Coherence length is important in holography and telecommunications engineering. Coherence length is usually applied to the optical regime.

In radio-band systems, the coherence length is approximated by,

$$L = \frac{c}{n\,\Delta f} = \frac{\lambda^2}{n\Delta\lambda},$$

Where c is the speed of light in vacuum, n is the refractive index of the medium, and Δf is the bandwidth of the source or λ is the signal wavelength and $\Delta\lambda$ is the width of the range of wavelengths in the signal.

The coherence length can be measured using a Michelson interferometer and is the optical path length difference of a self-interfering laser beam which corresponds to a $1/e = 37\%$ fringe visibility, where the fringe visibility is defined as,

$$V = \frac{I_{\max} - I_{\min}}{I_{\max} + I_{\min}},$$

Where I is the fringe intensity.

Multimode helium–neon lasers have a typical coherence length of 20 cm, while the coherence length of single-mode lasers can exceed 100 m. Semiconductor lasers reach some 100 m, but small, inexpensive semiconductor lasers have shorter lengths, with one source claiming 20 cm. Single mode fibre lasers with line widths of a few kHz can have coherence lengths exceeding 100 km. Similar coherence lengths can be reached with optical frequency combs due to the narrow line width of each tooth. Non-zero visibility is present only for short intervals of pulses repeated after cavity length distances up to this long coherence length.

NOTES

14.4 BCS THEORY AND COOPER PAIR

In 1957, the American physicists, John Bardeen, Leon N Cooper and John Robert Schrieffer proposed a microscopic theory (i.e., a quantum theory) to account for the observed properties of superconductors, which is known as BCS theory.

This theory involves the electron interactions through phonon as mediators (Figure 14.5). This theory is based on the formation of Cooper pairs which is purely a quantum mechanical concept.

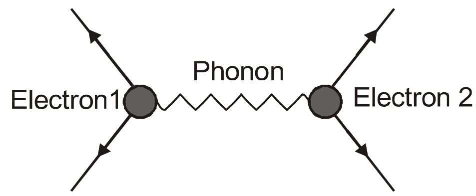


Fig. 14.5 *Electron-Lattice-Electron Interaction*

When an electron comes near a positive ion core of the lattice, it experiences an attractive force because of the opposite charge polarity between the electron and the ion core. Due to this interaction (electron-lattice interaction) the ion core will be displaced from its position which is called *lattice distortion*. The distortion causes an increase in the density of ions in the distorted region. The higher density of ions in the distorted region may attract an another electron. Thus, the second electron does not see the bare electron (i.e., the first electron) since it is screened by positive ions. Hence, the second electron will be attracted towards the first electron through the distorted lattice (lattice-electron interaction) which tends to reduce the energy of the first electron. Thus, this process is looked upon as an equivalent to the interaction between two electrons via the lattice. *Since the lattice vibrations are quantized in terms of phonons, the process is called electron-lattice-electron interaction via the phonon field. A pair of electrons thus coupled through a phonon is called a Cooper pair.*

Since there is a reduction of energy during the interaction, it is treated as equivalent to estabilishing an attractive force between the two electrons. This attractive force is maximum if the two electrons have equal and opposite spins and momentum.

At temperatures below the critical temperature ($T < T_c$) the attractive force dominates the usual coulombic repulsive force between the two electrons thus leading to the formation of Cooper pairs. At this stage, the Cooper pairs of electrons in materials do not encounter any scattering by the lattice points. As a result, the resistivity vanishes and the conductivity becomes very high (almost infinity) leading to superconducting state of the material.

The BCS theory is supported by the fact that, the good conductors such as Au, Ag and Cu do not exhibit superconductivity. The reason given is that, the electrons in these metals move so freely in the lattice that the electron lattice interaction is virtually absent. Thus, the possibility of formation of cooper pairs is negligible and, hence, the occurrence of superconductivity.

The distance among the lattice points in a superconductor upto which the cooper pair of electrons can maintain the coupled motion is called the coherent length. This is found to be of the order of 10^{-6}m.

The base of a quantum theory of superconductivity was put by the classic papers of Bardeen, Cooper, and Schrieffer in 1957. The "BCS theory of superconductivity" is applicable with a very wide range, from He atoms in their condensed phase, to type I and type II metallic superconductors. It is also applicable to superconductors based on planes of cuprite ions with high-temperature. After that, there is a "BCS wavefunction" which is composed of the particles in pairs k↓ and -k↓. If these are treated by the BCS theory then it gives the well-known electronic superconductivity which is observed in metals and exhibits the energy gaps shown in Table 3. This pairing is called as an s-wave pairing. There are certainly other forms of particle pairing which are possible with the BCS theory, but we do not need to consider here any forms other than the BCS wave-function. In this chapter, we are discussing the specific achievements of BCS theory with a BCS wavefunction, some of which are given below:

1. If there is an attractive interaction between electrons then it can separate ground state from excited states by an energy gap. The critical magnetic field, the thermal properties, and most of the electromagnetic properties are due to the energy gap.
2. The interaction of electron-lattice-electron can lead to an energy gap of a certain magnitude which can be observed. The indirect interaction takes place when one electron interacts with the lattice and deforms it. Then a second electron sees the deformed lattice and adapts itself to take advantage of the deformation to lower its energy. Hence, the second electron interacts with the first electron through the lattice deformation.
3. The penetration depth and the coherence length came out as natural consequences of the BCS theory. For magnetic fields that vary slowly in space, the London equation is obtained. So, the most important phenomenon in superconductivity called the Meissner effect is obtained naturally.
4. The transition temperature criteria of an element or alloy involves the electron density of orbitals $D(E_F)$ of one spin at the Fermi level and the electron-lattice interaction *U. This* can be estimated from the electrical resistivity as the resistivity at room temperature is an estimate of the electron-phonon interaction. For $UD(\varepsilon_F) << 1$ the BCS theory predicts that

$$T_c = 1.14\theta \exp[-1/UD(\varepsilon_F)] \qquad (14.1)$$

Where ¸ is the Debye temperature and U is an attractive interaction. The result for T_c is satisfied by the experimental data qualitatively. There is an interesting apparent anomaly that the higher the resistivity at room temperature the higher is U, and so, it is more likely that the metal will be a superconductor when cooled.

5. Magnetic flux obtained from a superconducting ring is quantized and the effective unit of charge is 2*e* instead of *e.* The ground state of BCS involves the pairs of electrons. Hence, the flux quantization in terms of the pair charge *2e* is an outcome of the theory.

BCS Ground State

The ground state of a Fermi gas of non-interacting electrons is the filled Fermi Sea. This state allows very small excitation. We can create an excited state by just taking an electron from the Fermi surface and putting it just above the Fermi surface. The BCS theory shows that if there is an appropriate attractive interaction between electrons then the new ground state is superconducting and it is separated by a finite energy gap E_g from its lowest excited state.

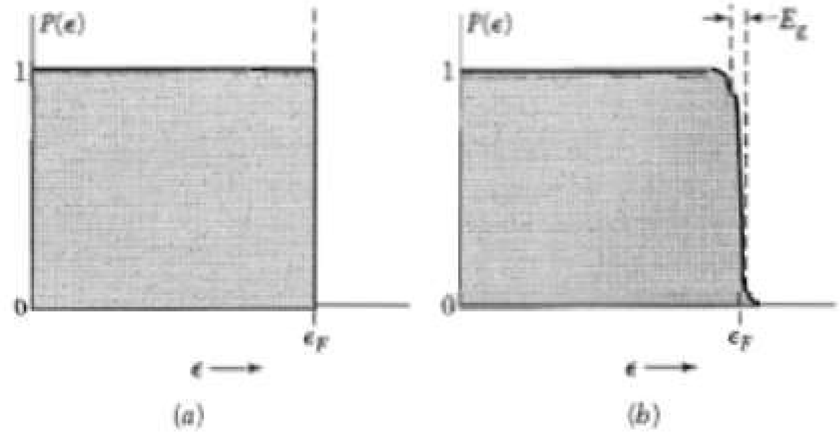


Fig. 14.6 *(a) Probability P that an Orbital of Kinetic Energy E is Occupied in the Ground State of the Noninteracting Fermi Gas; (b) the BCS Ground State Differs from the Fermi State in a Region of the Width of the Order of the Energy Gap Ep. Both Curves are for Absolute Zero.*

The formation of the BCS ground state is shown in Figure 14.6. The BCS state in (b) contains the mixtures of one-electron orbitals from above the Fermi energy T_F. At first look, the BCS state appears to have higher energy than the Fermi state. The comparison of (b) with (a) clearly shows that the kinetic energy of the BCS state is higher than that of the Fermi state. But the attractive potential energy of the BCS state, which is not represented in the figure reacts to lower the total energy of the BCS state in comparison to the Fermi state.

When the ground state of BCS of a many-electron system is defined in terms of the occupancy of one-particle orbitals. The orbitals which are near T_F are filled somewhat like a Fermi-Dirac distribution for some finite temperature.

The main feature of the BCS state is that the one-particle orbitals are occupied in the pairs that are if an orbital with wavevector k and spin up is occupied, then the orbital with wavevector -k and spin down is also occupied. 1f k↓ is vacant, then -k↓ is also vacant. These pairs are called Cooper pairs. They have zero spin and have many attributes of Bosons.

14.5 NORMAL TUNNELLING

Quantum tunnelling is the quantum mechanical phenomenon where a wavefunction can propagate through a potential barrier. The transmission through the barrier can be finite and depends exponentially on the barrier height and barrier width. The wavefunction may disappear on one side and reappear on the other side. The wavefunction and its first derivative are continuous. In steady-state, the probability flux in the forward direction is spatially uniform. No particle or wave is lost. Tunnelling occurs with barriers of thickness around 1–3 nm and smaller.

Tunnel Junction: A simple barrier can be created by separating two conductors with a very thin insulator. These are tunnel junctions, the study of which requires understanding quantum tunnelling. Josephson junctions take advantage of quantum tunnelling and the superconductivity of some semiconductors to create the Josephson effect. This has applications in precision measurements of voltages and magnetic fields, as well as the multijunction solar cell.

The Superconducting Tunnel Junction (STJ) — also known as a Superconductor–Insulator–Superconductor (SIS) tunnel junction— is an electronic device consisting of two superconductors separated by a very thin layer of insulating material. Current passes through the junction via the process of quantum tunnelling. The STJ is a type of Josephson junction, though not all the properties of the STJ are described by the Josephson effect.

These devices have a wide range of applications, including high-sensitivity detectors of electromagnetic radiation, magnetometers, high speed digital circuit elements, and quantum computing circuits.

All currents flowing through the STJ pass through the insulating layer via the process of quantum tunnelling. There are two components to the tunnelling current. The first is from the tunnelling of Cooper pairs. This supercurrent is described by the ac and dc Josephson relations, first predicted by Brian David Josephson in 1962.

The second is the quasiparticle current, which, in the limit of zero temperature, arises when the energy from the bias voltage eV exceeds twice the value of superconducting energy gap Ä. At finite temperature, a small quasiparticle tunnelling

current — called the subgap current — is present even for voltages less than twice the energy gap due to the thermal promotion of quasiparticles above the gap.

NOTES

If the STJ is irradiated with photons of frequency f the dc current-voltage curve will exhibit both Shapiro steps and steps due to photon-assisted tunnelling. Shapiro steps arise from the response of the supercurrent and occur at voltages equal to $nhf/(2e)$ where h is Planck's constant, e is the electron charge, and n is an integer. Photon-assisted tunnelling arises from the response of the quasiparticles and gives rise to steps displaced in voltage by nhf/e relative to the gap voltage.

14.6 HIGH TEMPERATURE SUPERCONDUCTORS

Based on the coolants to achieve superconductivity phenomena in materials, the superconductors fall in to two categories.

1. Low temperature superconductors.
2. High temperature superconductors.

Low Temperature Superconductors

Superconductors that require liquid helium as coolant are called as low temperature superconductors (LTS or Low – T_c*). Liquid helium temperature is 4.2 K above absolute zero.*

High Temperature Superconductors

Superconductors having their T_c *values above the temperature of liquid nitrogen (77 K or –196°C) are called the high temperature superconductors (HTS or High-*T_c*).*

After the discovery of superconducting in mercury (4K) by Heike Kammerling onnes, the critical temperature had been gradually increased from 4K of Hg to 23 K in the compound Nb_3Ge first discovered in 1973. This remained a record until 1986.

On January 27, 1986, a new era of superconductivity science and technology begin. J. George Bednorz and K.A. Muller using a variant of the materials synthesized by Michel, smashed the long-stand 23K temperature record with a compound of barium, lanthanum, copper and oxygen that at 30 K is a very indicator of superconductivity.

Similar materials with higher transition temperature (High-T_c) soon followed in the history of superconductors when $Y_1Ba_2Cu_3O_{7-\delta}$ (Y BCO) or the so called 1-2-3 compound was discovered in 1987. The 1-2-3 compound was the first oxide superconductor to have transition temperature above liquid nitrogen temperature.

Soon after the discovery of superconductivity in YBCO material, more than 50 superconducting cuprates are now known. Extensive research to find high-T_c superconductivity in other families of materials has been unsuccessful. The highest transition temperature currently known is 138 K in a thallium doped mercuric cuprate comprised of the elements Hg, Tl, Ba, Ca, Cu and oxygen.

Examples for high temperature superconductors are listed in Table 14.1

Table 14.1 *Examplefor High T_c Superconductors*

Material	T_c's in K
1. $Pb_2 YSr_2 Cu_3 O_8$	77
2. Y – Ba – Cu – O ($Y_1Ba_2 Cu_3 O_7$)	93 – 95
3. Tl (Bi) – Ba(Sr) – Ca – Cu – O	122 – 125
4. Hg – Ba – Ca – Cu – O	130 – 135

High T_c Superconducting Oxide

The structure of the most intensily studied high T_c material (1-2-3) is explained in brief in this section.

It is found that, the superconductivity in $Y_1 Ba_2 Cu_3 O_{7-x}$ system is due to $Y_1 Ba_2 Cu_3 O_7$ and its T_c is $\simeq$ 90 K. The detailed structural investigations by single crystal X-ray and neutron powder diffraction techniques have shown that $Y Ba_2 Cu_3 O_7$ is an orthorhombically distorted perovskite with a tripled cell along the c-axis as shown in Figure 14.6(a). The lattice parameters are a = 3.823 Å, b = 3.86 Å and c = 11.681 Å.

Substitutional studies on $Y_1 Ba_2 Cu_3 O_7$ have indicated that Y can be replaced by other magnetic rare earth, retaining the superconducting characteristics.

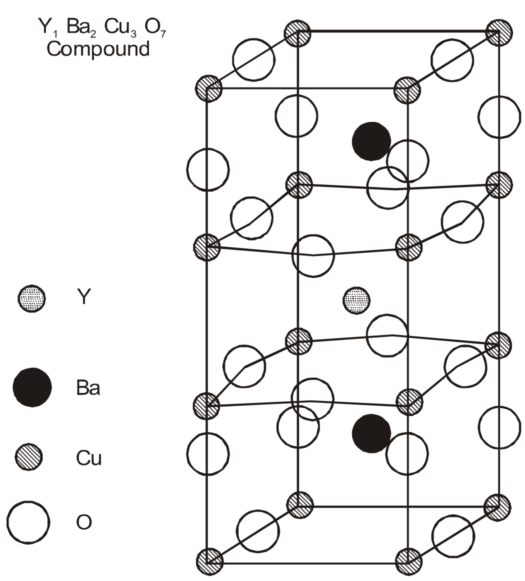


Fig. 14.6(a): *Structure of $Y_1 Ba_2 Cu_3 O_7$ Compound–Orthorhombic*

NOTES

Two more superconducting phases have been identified in the Y-Ba-Cu-O system having compositions $Y\ Ba_2\ Cu_3\ O_8$ and $Y_2\ Ba_4\ Cu_7\ O_{14}$ with $T_c \sim 80$ K and 40K respectively.

Neutron and X-ray diffraction measurements showed that, the orthorhombic to tetragonal phase transition in $Y\ Ba_2\ Cu_3\ O_{7-x}$ occurs above 700°C. T_c also drops down drastically in the range $x = 0.5 - 0.6$ and becomes zero at $x = 0.65$ and the structure changes to tetragonal symmetry whereby the superconductivity also disappears in the compound.

It was observed that, the decrease in the superconducting transition temperature is due to a disordering of the oxygen chains, which implies that the Cu-O chains play a major role in the mechanism for high temperature superconductivity.

The structure difference between the orthorhombic and tetragonal Figure 14.6(*b*) arises from the distribution of oxygen vacancies in the Cu(1) plane, i.e., in the tetragonal phase O_1 will be absent. One major advantage of high T_c superconductors is that, the liquid nitrogen can be used as a coolant to replace the more expensive liquid helium coolant.

The high temperature superconductors currently have only limited practical applications. The reason is, most of the high-T_c superconductors are ceramics which are brittle. But, in thin film technology these materials can find their applications in the electronic field such as high speed computers.

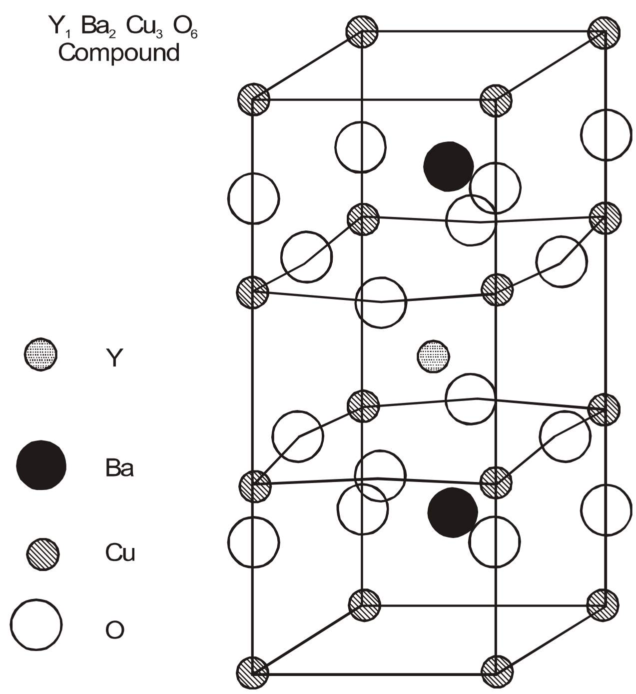


Fig. 14.6(b): *Structure of $Y_1\ Ba_2\ Cu_3\ O_6$ Compound–Tetragonal*

NOTES

Check Your Progress

1. What do you mean by the coherence length?
2. Elaborate on the BCS theory.
3. Illustrate the cooper pair.
4. Define the normal tunnelling.
5. Interpret the low temperature superconductors.
6. Explain the high temperature superconductors.

14.7 ANSWERS TO CHECK YOUR PROGRESS QUESTIONS

1. A major triumph of the equations of this theory is their ability to explain the Meissner effect, wherein a material exponentially expels all internal magnetic fields as it crosses the superconducting threshold. By using the London equation, one can obtain the dependence of the magnetic field inside the superconductor on the distance to the surface.
2. Magnetic levitation or maglev is the process by which an object is suspended above another object with no other support but magnetic fields. The phenomena of magnetic levitation is based on Meissner effect.
3. The magnetic levitation is brought about by enormous repulsion between two highly powerful magnetic fields.
4. The wave nature of moving particles makes the electrons to tunnel through the barrier (insulator), i.e., the electrons can tunnel from one superconductor to the other. As a consequence of the tunnelling of electrons (cooper pairs) across the insulator, there is a net current across the junction. This is called as Josephson effect.
5. Josephson junctions are used in sensitive magnetometers called SQUID-Superconducting Quantum Interference Device. SQUID detectors are used to measure the levels of iron in liver, so that iron built up can be treated before much harm is done to the body.
6. It is a relay or switch made of superconductors whose size can be made very small. In addition, these switches consume a very little current. The cryotron consists of two superconducting materials A and B.

NOTES

7. In condensed matter physics coherence length is the propagation distance over which a coherent wave (e.g., an electromagnetic wave) maintains a specified degree of coherence.
8. In 1957, the American physicists, John Bardeen, Leon N Cooper and John Robert Schrieffer proposed a microscopic theory (i.e., a quantum theory) to account for the observed properties of superconductors, which is known as BCS theory. This theory involves the electron interactions through phonon as mediators
9. Since the lattice vibrations are quantized in terms of phonons, the process is called electron- lattice- electron interaction via the phonon field. A pair of electrons thus coupled through a phonon is called a Cooper pair.
10. The Superconducting Tunnel Junction (STJ) — also known as a Superconductor–Insulator–Superconductor tunnel junction (SIS) — is an electronic device consisting of two superconductors separated by a very thin layer of insulating material.
11. Superconductors that require liquid helium as coolant are called as Low Temperature Superconductors (*LTS* or Low – Tc). Liquid helium temperature is 4.2 *K* above absolute zero.
12. Superconductors having their Tc values above the temperature of liquid nitrogen (77 *K* or –196°C) are called the High Temperature Superconductors (HTS or High- Tc).

14.8 SUMMARY

- A major triumph of the equations of this theory is their ability to explain the Meissner effect, wherein a material exponentially expels all internal magnetic fields as it crosses the superconducting threshold. By using the London equation, one can obtain the dependence of the magnetic field inside the superconductor on the distance to the surface.
- Magnetic levitation or maglev is the process by which an object is suspended above another object with no other support but magnetic fields. The phenomena of magnetic levitation is based on Meissner effect.
- The magnetic levitation is brought about by enormous repulsion between two highly powerful magnetic fields.
- The wave nature of moving particles makes the electrons to tunnel through the barrier (insulator), i.e., the electrons can tunnel from one superconductor to the other. As a consequence of the tunnelling of electrons (cooper pairs)

across the insulator, there is a net current across the junction. This is called as Josephson effect.

NOTES

- Josephson junctions are used in sensitive magnetometers called SQUID-Superconducting Quantum Interference Device. SQUID detectors are used to measure the levels of iron in liver, so that iron built up can be treated before much harm is done to the body.
- It is a relay or switch made of superconductors whose size can be made very small. In addition, these switches consume a very little current. The cryotron consists of two superconducting materials A and B.
- In condensed matter physics coherence length is the propagation distance over which a coherent wave (e.g. an electromagnetic wave) maintains a specified degree of coherence.
- In 1957, the American physicists, John Bardeen, Leon N Cooper and John Robert Schrieffer proposed a microscopic theory (i.e., a quantum theory) to account for the observed properties of superconductors, which is known as BCS theory. This theory involves the electron interactions through phonon as mediators.
- Since the lattice vibrations are quantized in terms of phonons, the process is called electron- lattice- electron interaction via the phonon field. A pair of electrons thus coupled through a phonon is called a Cooper pair.
- Quantum tunnelling is the quantum mechanical phenomenon where a wavefunction can propagate through a potential barrier. The transmission through the barrier can be finite and depends exponentially on the barrier height and barrier width.
- A simple barrier can be created by separating two conductors with a very thin insulator. These are tunnel junctions, the study of which requires understanding quantum tunnelling.
- Josephson junctions take advantage of quantum tunnelling and the superconductivity of some semiconductors to create the Josephson effect. This has applications in precision measurements of voltages and magnetic fields, as well as the multijunction solar cell.
- The Superconducting Tunnel Junction (STJ) — also known as a Superconductor–Insulator–Superconductor tunnel junction (SIS) — is an electronic device consisting of two superconductors separated by a very thin layer of insulating material.
- Superconductors that require liquid helium as coolant are called as Low Temperature Superconductors (*LTS* or Low – T_c). Liquid helium temperature is 4.2 *K* above absolute zero.

- Superconductors having their T_c values above the temperature of liquid nitrogen (77 K or –196°C) are called the High Temperature Superconductors (HTS or High- T_c).

NOTES

14.9 KEY WORDS

- **London equations:** A major triumph of the equations of this theory is their ability to explain the Meissner effect, wherein a material exponentially expels all internal magnetic fields as it crosses the superconducting threshold.
- **Josephson effect:** The wave nature of moving particles makes the electrons to tunnel through the barrier (insulator), i.e., the electrons can tunnel from one superconductor to the other. As a consequence of the tunnelling of electrons (cooper pairs) across the insulator, there is a net current across the junction. This is called as Josephson effect.
- **Coherence length:** In condensed matter physics coherence length is the propagation distance over which a coherent wave (e.g. an electromagnetic wave) maintains a specified degree of coherence.
- **BCS theory:** This theory involves the electron interactions through phonon as mediators.
- **Cooper pair:** Since the lattice vibrations are quantized in terms of phonons, the process is called electron-lattice-electron interaction via the phonon field. A pair of electrons thus coupled through a phonon is called a Cooper pair.
- **High temperature superconductors:** Superconductors having their T_c values above the temperature of liquid nitrogen (77 K or –196°C) are called the High Temperature Superconductors (HTS or High- T_c).

14.10 SELF ASSESSMENT QUESTIONS AND EXERCISES

Short-Answer Questions

1. Interpret the London equations.
2. Explain the magnetic levitation.
3. Define the Josephson effect.
4. What do you mean by the cryotron?
5. Illustrate the coherence length.

NOTES

6. State the BCS theory.
7. Elaborate on the Cooper pair.
8. Explain the normal tunnelling.
9. Define the low temperature superconductors.
10. What is high temperature superconductors?

Long-Answer Questions

1. Briefly define the London equations with the help of examples.
2. Describe the coherence length.
3. Analyse the BCS theory and Cooper pair.
4. Discuss briefly the normal tunnelling. Give appropriate examples.
5. Explain the high temperature superconductors.

14.11 FURTHER READINGS

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